CSCI567 Machine Learning (Fall 2025)

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Sep 19, 2025

Administration

Will discuss HW1 solutions in today discussion session.

HW2 will be released next week.

Outline

1. Review of Last Lecture
2. Multiclass Classification
3. Kernel methods

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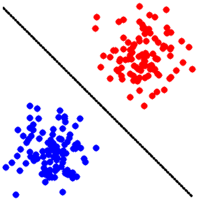
Linear classifiers

Linear models for **binary** classification:

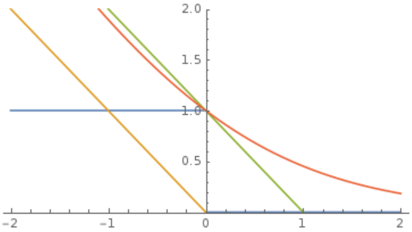
Step 1. Model is the set of **separating hyperplanes**

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



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:** $\boldsymbol{w} \leftarrow \boldsymbol{w} - \left(\nabla^2 F(\boldsymbol{w})\right)^{-1} \nabla F(\boldsymbol{w})$

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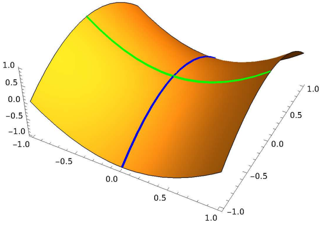
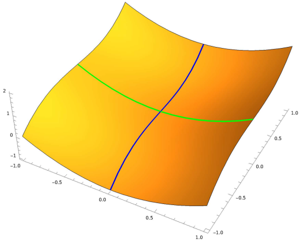
- for convex objectives, this is all we need
- for nonconvex objectives, can get stuck at local minimizers or “bad” saddle points (random initialization escapes “good” saddle points)



“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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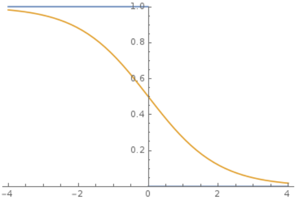
Repeat:

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

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



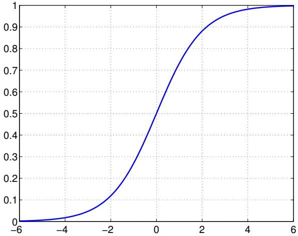
A Probabilistic view of logistic regression

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

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



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1. Review of Last Lecture
2. Multiclass Classification
   - Multinomial logistic regression
   - Reduction to binary classification
3. Kernel methods

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:

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- predicting weather: sunny, cloudy, rainy, etc
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Nearest Neighbor Classifier naturally works for arbitrary C.

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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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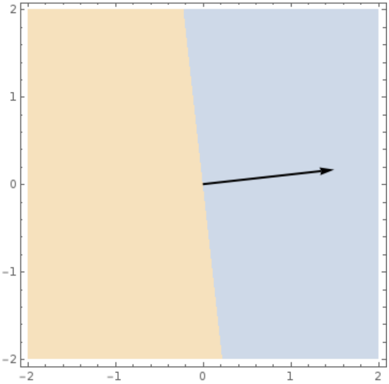

$$\boldsymbol{w} = \left(\tfrac{3}{2}, \tfrac{1}{6}\right)$$

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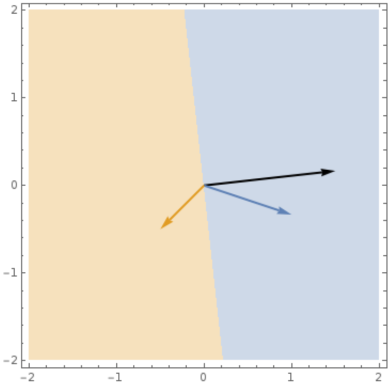

$\boldsymbol{w} = (\frac{3}{2}, \frac{1}{6}) = \boldsymbol{w}_1 - \boldsymbol{w}_2$
$\boldsymbol{w}_1 = (1, -\frac{1}{3})$
$\boldsymbol{w}_2 = (-\frac{1}{2}, -\frac{1}{2})$

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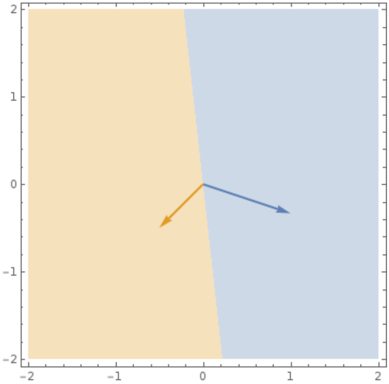

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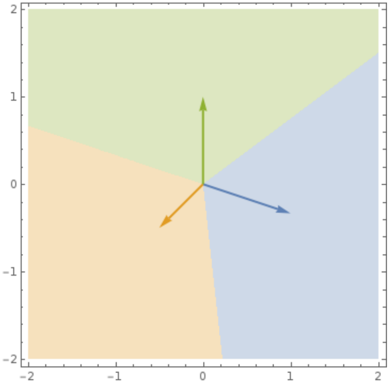

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- Green class: $\{\boldsymbol{x} : 3 = \mathrm{argmax}_k\, \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}\}$

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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Important operator: *softmax function* (or really, "softargmax")

For a vector $s \in \mathbb{R}^{\mathsf{C}}$, softmax$(s) = \left(\frac{e^{s_1}}{\sum_{k \in [\mathsf{C}]} e^{s_k}}, \cdots, \frac{e^{s_{\mathsf{C}}}}{\sum_{k \in [\mathsf{C}]} e^{s_k}} \right)$

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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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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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If $k \neq y_n$:

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

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

Step 3: Optimization

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

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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

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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 drawn from $\mathrm{softmax}(\boldsymbol{W}\boldsymbol{x})$

Generalization of cross-entropy loss

Given a general model class:

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

where $s : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}^{\mathsf{C}}$ is a **"scoring" function**.

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

$$-\ln\left(\text{softmax}(s(\boldsymbol{x}))_y\right) = -\ln\left(\frac{e^{s(\boldsymbol{x})_y}}{\sum_{k\in[\mathsf{C}]} e^{s(\boldsymbol{x})_k}}\right) = \ln\left(1 + \sum_{k\neq y} e^{s(\boldsymbol{x})_k - s(\boldsymbol{x})_y}\right)$$

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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.)
- **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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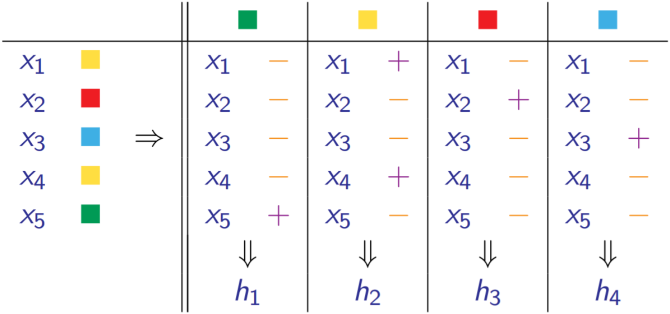

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Issue: will (probably) make a mistake *as long as one of h_k errs*.

One-versus-one (OvO)

(picture credit: link)

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'),

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- *discard all other examples*
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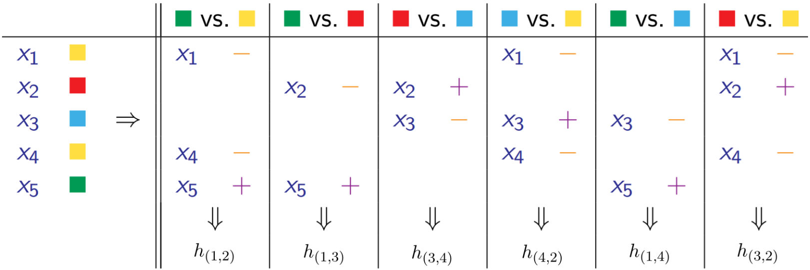

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Prediction: for a new example $\boldsymbol{x}$

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

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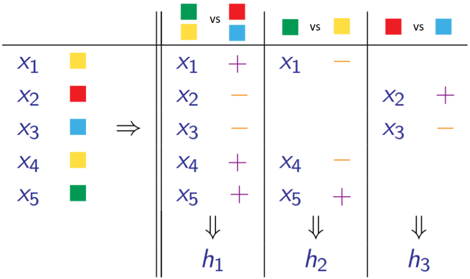
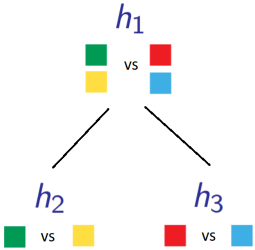
Training: see pictures





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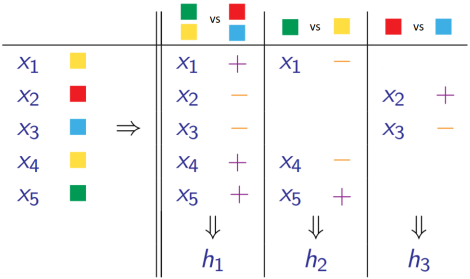

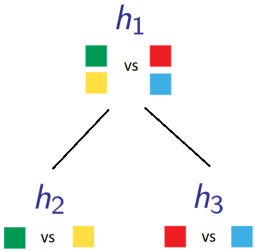

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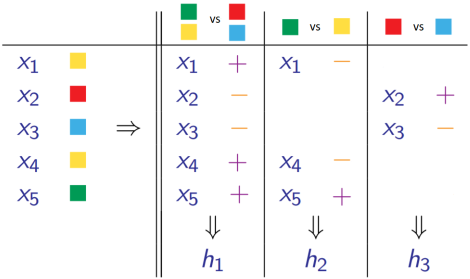

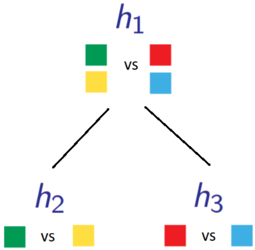

Prediction is also natural, *but is very fast!* (think ImageNet where $C \approx 20K$)

Comparisons

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

training time: how many training points are created

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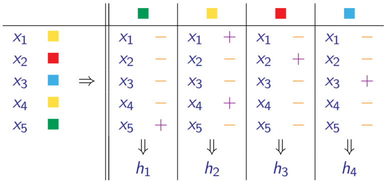

Comparisons

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

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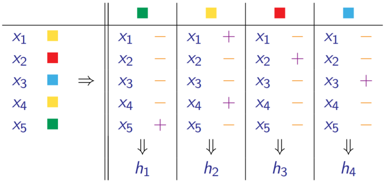

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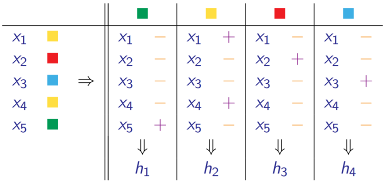

Comparisons

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

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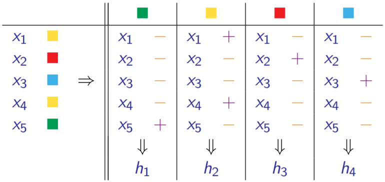

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Reduction	**training time**	**prediction time**	**remark**
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OvO			

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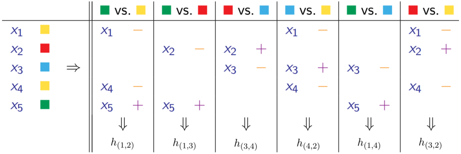

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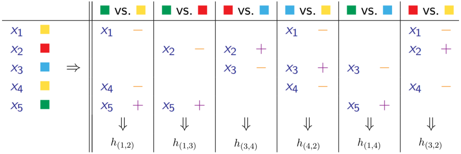

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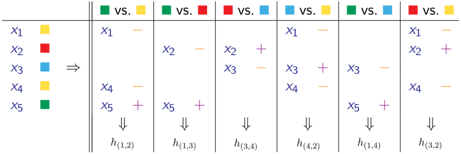

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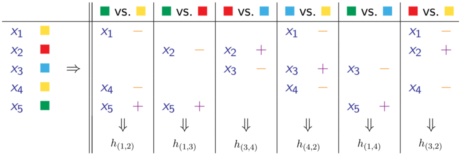

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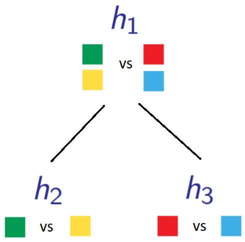

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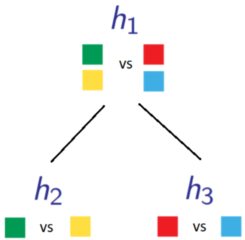

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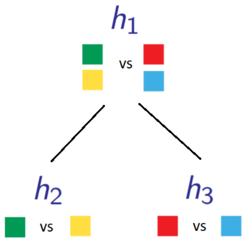

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Tree	$\mathcal{O}((\log_2 \mathsf{C})\mathsf{N})$	$\mathcal{O}(\log_2 \mathsf{C})$	good for "extreme classification"

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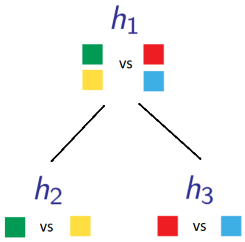

Outline

1. Review of Last Lecture
2. Multiclass Classification
3. Kernel methods
   - Motivation
   - Example: Perceptron
   - Kernel Trick
   - Kernelized Perceptron

Motivation

Recall: when linear models are not good enough, we can use **a nonlinear feature map** $\phi : \mathbb{R}^{\mathsf{D}} \rightarrow \mathbb{R}^{\mathsf{M}}$ to transform all $\boldsymbol{x}$ to $\phi(\boldsymbol{x})$.

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Issue: what if M is huge, or even infinity?

Solution: **kernel methods**

Case study: Perceptron for binary classification

Perceptron

Initialize $\boldsymbol{w} = \boldsymbol{0}$

Repeat:

- Pick a data point index n uniformly at random
- If $\text{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n) \neq y_n$, update $\boldsymbol{w} \leftarrow \boldsymbol{w} + y_n\boldsymbol{x}_n$

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where $\alpha_m = y_m \times$ number of times x_m has been misclassified

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How to update $\alpha_1, \ldots, \alpha_{\mathsf{N}}$ so that $\sum_{m=1}^{\mathsf{N}} \alpha_m \boldsymbol{x}_m \equiv \boldsymbol{w}$ holds always?

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Applying a feature map

Perceptron (primal form with ϕ)

Initialize $\boldsymbol{w} = \mathbf{0} \in \mathbb{R}^{\mathsf{M}}$
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If we can compute $\boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)$ without explicitly evaluating $\boldsymbol{\phi}(\boldsymbol{x}_m)$ and $\boldsymbol{\phi}(\boldsymbol{x}_n)$, then time/space is independent of M!

Example

Consider the following polynomial basis $\phi : \mathbb{R}^2 \to \mathbb{R}^3$:

$$\boldsymbol{\phi}(\boldsymbol{x}) = \begin{pmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{pmatrix}$$

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Therefore, *the inner product in the new space is simply a function of the inner product in the original space*.

Another example

$\boldsymbol{\phi} : \mathbb{R}^{\mathsf{D}} \rightarrow \mathbb{R}^{2\mathsf{D}}$ is parameterized by θ:

$$\boldsymbol{\phi}_\theta(\boldsymbol{x}) = \begin{pmatrix} \cos(\theta x_1) \\ \sin(\theta x_1) \\ \vdots \\ \cos(\theta x_{\mathsf{D}}) \\ \sin(\theta x_{\mathsf{D}}) \end{pmatrix}$$

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Once again, *the inner product in the new space is a simple function of the features in the original space*.

More complicated example

Based on ϕ_θ, define $\phi_L : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}^{2\mathsf{D}(L+1)}$ for some integer L:

$$\boldsymbol{\phi}_L(\boldsymbol{x}) = \begin{pmatrix} \boldsymbol{\phi}_0(\boldsymbol{x}) \\ \boldsymbol{\phi}_{\frac{2\pi}{L}}(\boldsymbol{x}) \\ \boldsymbol{\phi}_{2\frac{2\pi}{L}}(\boldsymbol{x}) \\ \vdots \\ \boldsymbol{\phi}_{L\frac{2\pi}{L}}(\boldsymbol{x}) \end{pmatrix}$$

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What is the inner product between $\boldsymbol{\phi}_L(\boldsymbol{x})$ and $\boldsymbol{\phi}_L(\boldsymbol{x}')$?

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Infinite dimensional mapping

When $L \to \infty$, even if we cannot compute $\phi(x)$, a vector of *infinite dimension*, we can still compute inner product:

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Note that using this mapping in linear classification, we are *learning a weight $\boldsymbol{w}$ with infinite dimension!*

Kernel functions

Definition: a function $k : \mathbb{R}^{\mathsf{D}} \times \mathbb{R}^{\mathsf{D}} \rightarrow \mathbb{R}$ is called a *kernel function* if there exists a function $\boldsymbol{\phi} : \mathbb{R}^{\mathsf{D}} \rightarrow \mathbb{R}^{\mathsf{M}}$ so that for any $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{\mathsf{D}}$,

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Examples we have seen

$$k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^{\mathrm{T}} \boldsymbol{x}')^2$$

$$k(\boldsymbol{x}, \boldsymbol{x}') = \sum_{d=1}^{\mathsf{D}} \frac{\sin(2\pi(x_d - x'_d))}{x_d - x'_d}$$

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Creating more kernel functions using the following rules:

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- $\cdots$

Verify using the definition of kernel!

Common kernel functions

Two most commonly used kernel functions in practice:

Polynomial kernel

$$k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}' + c)^d$$

for $c \geq 0$ and d is a positive integer.

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Think about *what the corresponding ϕ is* for each kernel.

Back to Perceptron

Perceptron (dual form with $\boldsymbol{\phi}$)

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Kernelized Perceptron

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- If $\operatorname{sgn}(\sum_{m=1}^{\mathsf{N}} \alpha_m k(\boldsymbol{x}_m, \boldsymbol{x}_n)) \neq y_n$, update $\alpha_n \leftarrow \alpha_n + y_n$

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Completely M-*independent*, becomes a *non-parametric* method

Gram/kernel matrix

When N is small, can precompute all inner products as a **Gram matrix**

$$\boldsymbol{K} = \begin{pmatrix} k(\boldsymbol{x}_1, \boldsymbol{x}_1) & k(\boldsymbol{x}_1, \boldsymbol{x}_2) & \cdots & k(\boldsymbol{x}_1, \boldsymbol{x}_N) \\ k(\boldsymbol{x}_2, \boldsymbol{x}_1) & k(\boldsymbol{x}_2, \boldsymbol{x}_2) & \cdots & k(\boldsymbol{x}_2, \boldsymbol{x}_N) \\ \vdots & \vdots & \vdots & \vdots \\ k(\boldsymbol{x}_N, \boldsymbol{x}_1) & k(\boldsymbol{x}_N, \boldsymbol{x}_2) & \cdots & k(\boldsymbol{x}_N, \boldsymbol{x}_N) \end{pmatrix}$$

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Recall: $\boldsymbol{\Phi} = \begin{pmatrix} \boldsymbol{\phi}(\boldsymbol{x}_1)^{\mathrm{T}} \\ \boldsymbol{\phi}(\boldsymbol{x}_2)^{\mathrm{T}} \\ \vdots \\ \boldsymbol{\phi}(\boldsymbol{x}_N)^{\mathrm{T}} \end{pmatrix} \in \mathbb{R}^{N \times M}$

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Gram matrix vs covariance matrix

	dimensions	entry (i, j)	property
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Gram matrix vs covariance matrix

	dimensions	entry (i, j)	property
$\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}}$	N × N	$\boldsymbol{\phi}(\boldsymbol{x}_i)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_j)$	both are **symmetric** and **positive semidefinite**
$\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}$	M × M	$\sum_{n=1}^{N} \phi(\boldsymbol{x}_n)_i \phi(\boldsymbol{x}_n)_j$	

Mercer Theorem

$k : \mathbb{R}^\mathsf{D} \times \mathbb{R}^\mathsf{D} \rightarrow \mathbb{R}$ is a kernel function if and only if the Gram matrix $\boldsymbol{K}$ for *any N and any $\boldsymbol{x}_1$, $\boldsymbol{x}_2$, . . ., $\boldsymbol{x}_N$* is positive semidefinite.

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$$k(\boldsymbol{x}, \boldsymbol{x}') = \|\boldsymbol{x} - \boldsymbol{x}'\|_2^2$$

is *not a kernel*, why?

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If it is a kernel, the kernel matrix for two data points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$:

$$\boldsymbol{K} = \begin{pmatrix} 0 & \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_2^2 \\ \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_2^2 & 0 \end{pmatrix}$$

must be positive semidefinite,

Mercer Theorem

$k : \mathbb{R}^{\mathsf{D}} \times \mathbb{R}^{\mathsf{D}} \rightarrow \mathbb{R}$ is a kernel function if and only if the Gram matrix $\boldsymbol{K}$ for *any N and any $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N$* is positive semidefinite.

- useful for showing that a function is not a kernel

Example:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \|\boldsymbol{x} - \boldsymbol{x}'\|_2^2$$

is *not a kernel*, why?

If it is a kernel, the kernel matrix for two data points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$:

$$\boldsymbol{K} = \begin{pmatrix} 0 & \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_2^2 \\ \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_2^2 & 0 \end{pmatrix}$$

must be positive semidefinite, but it is not (contradiction).

Kernelizing ML algorithms

Many other ML algorithms can be **kernelized**:

- nearest neighbor classifier
- linear regression
- logistic regression
- SVM
- $\cdots$

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Key idea: rewrite the algorithm so that its dependence on the transformed dataset $\mathbf{\Phi}$ is only through the Gram matrix $\boldsymbol{K} = \mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}$.