CSCI-567: Machine Learning (Fall 2019)

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Outline

Outline

Regression

Predicting a continuous outcome variable using past observations

Key difference from classification

- continuous vs discrete
- measure *prediction errors* differently.
- lead to quite different learning algorithms.

Linear Regression: regression with *linear models:* $f(\boldsymbol{w}) = \boldsymbol{w}^T\boldsymbol{x} = \boldsymbol{x}^T\boldsymbol{w}$

Linear Least Squares Regression

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{n=1}^{N} (\boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{w} - y_n)^2 = \underset{\boldsymbol{w}}{\operatorname{argmin}} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2$$

Three approaches to find the minimum:

- Closed Form (setting gradient to zero) $\boldsymbol{w}^* = \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{y}$
- Gradient Descent (GD)
- Stochastic Gradient Descent (SGD)

Gradient

The gradient vector ∇f points in the direction of greatest rate of increase of f at a given point.

The the rates of change of f in all directions is given by

$$\nabla f \cdot u = \|\nabla f\| \|u\| \cos\alpha$$

Hence, the direction of *greatest decrease* of f is the direction opposite to the gradient vector, when $\alpha = \pi$

We will minimize $RSS(w)$ using a gradient descent method.

Gradient Descent (GD)

Goal: minimize $f(w)$

Consider the definition

$$f'(w) = \lim_{\Delta x \to 0} \frac{f(w + \Delta x) - f(w)}{\Delta x}$$

Our gradient is an estimation of the derivative

$$\nabla f(w) = \frac{f(w + \Delta x) - f(w)}{\Delta x}$$

Then we need to move in its *opposite* direction to climb down the function.

$$f(w + \Delta x) = f(w) - \Delta x \nabla f(w)$$

Algorithm: Gradient Descent

Goal: minimize $F(\boldsymbol{w})$

Algorithm: move a bit in the *negative gradient direction*

initialize $\boldsymbol{w}^{(0)}$
while not converged do

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \lambda \nabla F(\boldsymbol{w}^{(t)})$$

where $\lambda > 0$ is called *step size or learning rate*

- *in theory λ should be set in terms of some parameters of F*
- *in practice we just try several small values*
- *there are many possible ways to detect convergence.*

An example

Example: $F(\boldsymbol{w}) = 0.5(w_1^2 - w_2)^2 + 0.5(w_1 - 1)^2$.
Gradient is

$$\frac{\partial F}{\partial w_1} = 2(w_1^2 - w_2)w_1 + w_1 - 1 \qquad \frac{\partial F}{\partial w_2} = -(w_1^2 - w_2)$$

GD:

- Initialize $w_1^{(0)}$ and $w_2^{(0)}$ (to be 0 or *randomly*), $t = 0$
- do

$$w_1^{(t+1)} \leftarrow w_1^{(t)} - \lambda \left[2({w_1^{(t)}}^2 - w_2^{(t)})w_1^{(t)} + w_1^{(t)} - 1 \right]$$
$$w_2^{(t+1)} \leftarrow w_2^{(t)} - \lambda \left[-({w_1^{(t)}}^2 - w_2^{(t)}) \right]$$
$$t \leftarrow t + 1$$

- until $F(\boldsymbol{w}^{(t)})$ **does not change much**

Why GD?

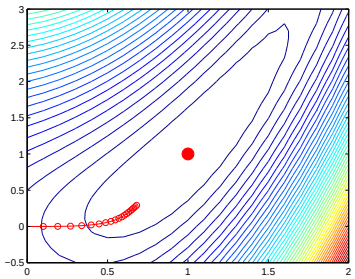
Using the first-order approximation

$$f(w + \Delta x) = f(w) + \Delta x \nabla f(w)$$

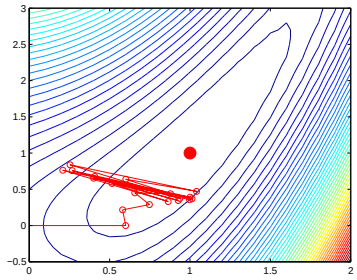
we move a bit in the negative gradient direction $\Delta x = -\lambda \nabla f(w)$

This ensures

$$f(w - \lambda \nabla f(w)) = f(w) - \lambda (\nabla f(w))^2 \leq f(w)$$



reasonable λ decreases function value



but large λ is unstable

Applying GD to Linear Regression

In the previous discussion, we have computed:

$$\frac{1}{2}\nabla RSS(\boldsymbol{w}) = \boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\boldsymbol{w} - \boldsymbol{X}^{\mathrm{T}}\boldsymbol{y} = \sum_n \boldsymbol{x}_n(\boldsymbol{x}_n^{\mathrm{T}}\boldsymbol{w} - y_n) = \sum_n \boldsymbol{x}_n(f(\boldsymbol{x}_n) - y_n)$$

GD update:

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \lambda \boldsymbol{X}^{\mathrm{T}} \left(\boldsymbol{X}\boldsymbol{w}^{(t)} - \boldsymbol{y} \right)$$

For a single weight,

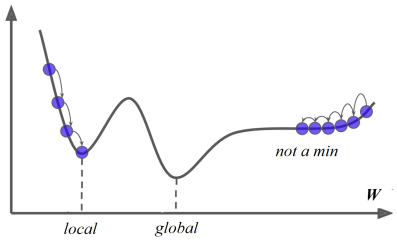
$$w_j^{(t+1)} \leftarrow w_j^{(t)} - \lambda \sum_n x_{nj} \left(f(\boldsymbol{x}_n) - y_n \right)$$

The algorithm uses all training points on each iteration. The algorithm is called *batch gradient descent*.

GD challenges

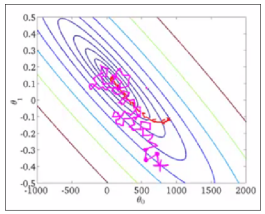
There two main challenges with GD:

- it may converge to a local minimum.
- it may not find a minimum at all. "vanishing gradient".



Stochastic Gradient Descent (SGD)

- GD: move a bit in the negative gradient direction.
- SGD: move a bit in a *noisy* negative gradient direction.
- In SGD, we use one training sample at each iteration.
- Need to randomly shuffle the training examples before calculating it.
- SGD is widely used for larger dataset and can be trained in parallel.



SGD for Linear Regression

Algorithm:

initialize $\boldsymbol{w}^{(0)}$
for each training sample n**:**
  for each weight j**:**

$$w_j^{(t+1)} \leftarrow w_j^{(t)} - \lambda\, x_{nj}\left(f(\boldsymbol{x}_n) - y_n\right)$$

The term "stochastic" comes from the fact that the gradient based on a single training sample.

SGD makes progress with each training example as it looks at.

Key point: it could be *much faster to obtain a stochastic gradient*!

GD versus SGD

In GD we calculate the gradient for all training points

In SGD we calculate the gradient for one sample (or a small batch, called a *mini-batch*) of training data

In SGD you might not be taking the most optimal route to get to the solution.

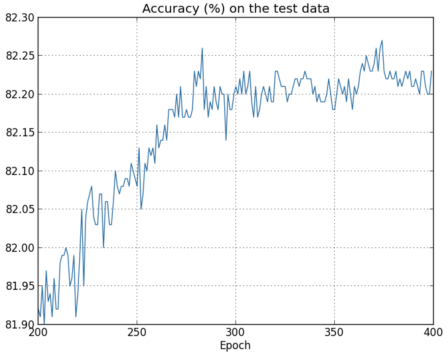
SGD may work for non-convex functions

In SGD you need to go through the training set several times (this is called an *epoch*).

You must specify the batch size (a typical size is 256) and number of epochs (a hyperparameter) for a learning algorithm.

Epoch and overfitting

This shows how test accuracy is changing due to the number of epochs:



Outline

General idea to provide ML algorithms

1. Pick a set of **models** $\mathcal{F}$
   - e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$
2. Define **error/loss** $L(y', y)$
3. Find **empirical risk minimizer (ERM)**:

$$\boldsymbol{f}^* = \operatorname*{argmin}_{f \in \mathcal{F}} \sum_{n=1}^{N} L(f(x_n), y_n)$$

Deriving classification algorithms

Let's follow the steps:

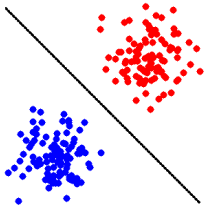
Step 1. Pick a set of models $\mathcal{F}$.

Again try linear models, but how to predict a label using $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$?

Sign of $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ predicts the label:

$$\text{sign}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) = \begin{cases} +1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} > 0 \\ -1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \leq 0 \end{cases}$$

(Sometimes use sgn for sign too.)



The models

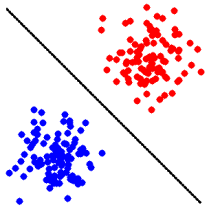
The set of **(separating) hyperplanes**:

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

Good choice for *linearly separable* data, i.e., $\exists \boldsymbol{w}$ s.t.

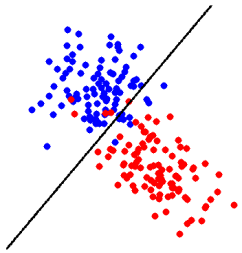
$$\text{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x_n}) = y_n \quad \text{or} \quad y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x_n} > 0$$

for all $n \in [N]$.



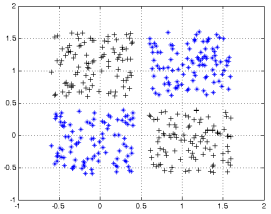
The models

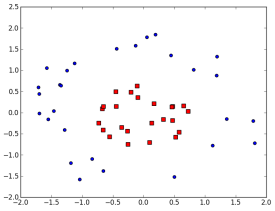
Still makes sense for "almost" linearly separable data



The models

For clearly not linearly separable data,





Again can apply a **nonlinear mapping** $\boldsymbol{\Phi}$:

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

More discussions in the next lectures.

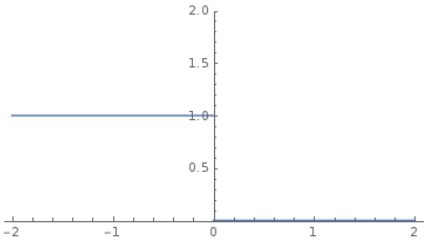
0-1 Loss

Step 2. Define error/loss $L(y', y)$.

Most natural one for classification: **0-1 loss** $L(y', y) = \mathbb{I}[y' \neq y]$

For classification, more convenient to look at the loss **as a function of** $y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$. That is, with

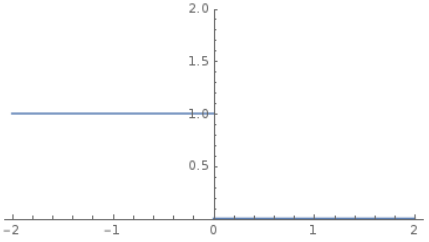
$$\ell_{0\text{-}1}(z) = \mathbb{I}[z \leq 0]$$



the loss for hyperplane $\boldsymbol{w}$ on example $(\boldsymbol{x}, y)$ is $\ell_{0\text{-}1}(y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$

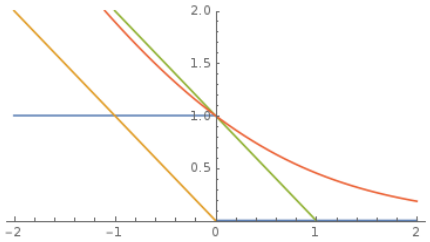
Minimizing 0-1 loss is hard

However, 0-1 loss is *not convex*.



Even worse, minimizing 0-1 loss is *NP-hard in general*. Recall Integer Linear programming.

Surrogate Losses



- 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)

ML becomes convex optimization

Step 3. Find ERM:

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

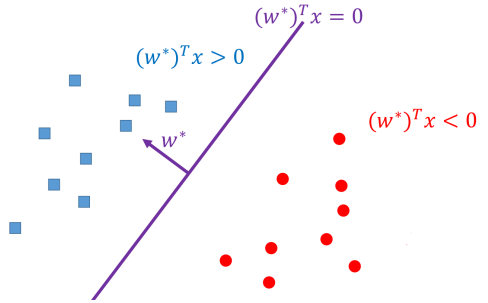
where $\ell(\cdot)$ can be perceptron/hinge/logistic loss

- *no closed-form* in general (unlike linear regression)
- can apply general convex optimization methods

Outline

The Perceptron

The Perceptron (introduced by Rosenblatt in 1957) is a linear model for classification. Its model is a hyperplane that partitions space into two regions. Perceptron is a rough model for how individual neurons in the brain work.



The Perceptron Algorithm

Mathematically: Stochastic Gradient Descent applied to perceptron loss

i.e. find the minimizer of

$$F(\boldsymbol{w}) = \sum_{n=1}^{N} \ell_{\text{perceptron}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$
$$= \sum_{n=1}^{N} \max\{0, -y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n\}$$

using SGD

Applying GD to perceptron loss

Objective

$$F(\boldsymbol{w}) = \sum_{n=1}^{N} \max\{0, -y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n\}$$

Gradient is

$$\nabla F(\boldsymbol{w}) = \sum_{n=1}^{N} -\mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

(only misclassified examples contribute to the gradient)

GD update

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \lambda \sum_{n=1}^{N} \mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

Applying SGD to perceptron loss

How to construct a stochastic gradient?

SGD update

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \lambda \mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

The Perceptron Algorithm

Perceptron algorithm is *SGD with* $\lambda = 1$ *applied to perceptron loss:*

Repeat:

- *Pick a data point* $\boldsymbol{x}_n$ *uniformly at random*
- *If* $\text{sgn}(\boldsymbol{w}^T \boldsymbol{x}_n) \neq y_n$

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + y_n \boldsymbol{x}_n$$

Note:

- *The algorithm is online and error driven.*
- *If the prediction is correct, it does nothing.*
- $\boldsymbol{w}$ *is always a linear combination of the training examples.*
- *It uses epochs as a hyperparameter.*

Why does it make sense?

If the current weight $\boldsymbol{w}$ makes a mistake

$$y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n < 0$$

then after the update $\boldsymbol{w}' = \boldsymbol{w} + y_n \boldsymbol{x}_n$ we have

$$y_n \boldsymbol{w}'^{\mathrm{T}} \boldsymbol{x}_n = y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n + y_n^2 \boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{x}_n = y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n + \|\boldsymbol{x}_n\|^2 \geq y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n$$

Thus it is more likely to get it right after the update.

Any theory?

- If training set is linearly separable, Perceptron *converges in a finite number of steps*
- How long does it take to converge?
- By "how long", what we really mean is "how many updates".
- One way to make this definition is through the notion of margin.
- The margin is the distance between the hyperplane and the nearest point.

Perceptron Convergence Theorem

Suppose the perceptron algorithm is run on a linearly separable data set $\mathcal{D}$ with margin $\gamma \geq 0$. Assume that $\|x\| = 1$. Then the algorithm will converge after at most $\frac{1}{\gamma^2}$ updates.

Outline

A simple view

In one sentence: find the minimizer of

$$F(\boldsymbol{w}) = \sum_{n=1}^{N} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$
$$= \sum_{n=1}^{N} \ln(1 + e^{-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n})$$

But why logistic loss? and why "regression"?

Predicting probability

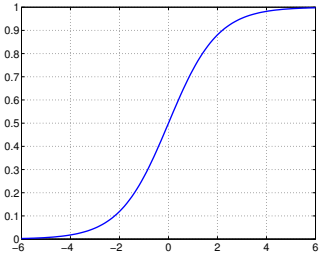
Instead of predicting a discrete label, can we *predict the probability of each label?* i.e. regress the probabilities

One way: **sigmoid function + linear model**

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

where σ is the sigmoid function:

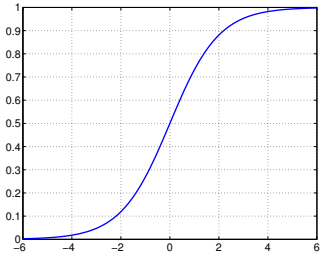
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$



Properties

Properties of sigmoid $\sigma(z) = \frac{1}{1+e^{-z}}$

- between 0 and 1 (good as probability)
- $\sigma(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}) \geq 0.5 \Leftrightarrow \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x} \geq 0$, consistent with predicting the label with $\text{sgn}(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x})$
- larger $\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x} \Rightarrow$ larger $\sigma(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}) \Rightarrow$ higher *confidence* in label 1
- $\sigma(z) + \sigma(-z) = 1$ for all z



The probability of label -1 is naturally

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

and thus

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

How to regress with discrete labels?

What we observe are labels, not probabilities.

Take a **probabilistic view**

- assume data is generated in this way by some $\boldsymbol{w}$
- perform Maximum Likelihood Estimation (MLE)

Specifically, what is the probability of seeing label $y_1, \cdots, y_n$ given $x_1, \cdots, x_n$, as a function of some $\boldsymbol{w}$?

$$P(\boldsymbol{w}) = \prod_{n=1}^{N} \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w})$$

MLE: find $\boldsymbol{w}^*$ that **maximizes the probability** $P(w)$

The MLE solution

$$\begin{aligned}\boldsymbol{w}^* &= \operatorname*{argmax}_{\boldsymbol{w}} P(\boldsymbol{w}) = \operatorname*{argmax}_{\boldsymbol{w}} \prod_{n=1}^{N} \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w}) \\ &= \operatorname*{argmax}_{\boldsymbol{w}} \sum_{n=1}^{N} \ln \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w}) = \operatorname*{argmin}_{\boldsymbol{w}} \sum_{n=1}^{N} -\ln \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w}) \\ &= \operatorname*{argmin}_{\boldsymbol{w}} \sum_{n=1}^{N} \ln(1 + e^{-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x_n}}) = \operatorname*{argmin}_{\boldsymbol{w}} \sum_{n=1}^{N} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) \\ &= \operatorname*{argmin}_{\boldsymbol{w}} F(\boldsymbol{w})\end{aligned}$$

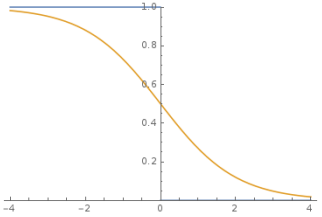
i.e. *minimizing logistic loss is exactly doing MLE for the sigmoid model!*

Let's apply SGD again

$$\begin{aligned}\boldsymbol{w} &\leftarrow \boldsymbol{w} - \lambda \nabla F(\boldsymbol{w}) \\ &= \boldsymbol{w} - \lambda \nabla_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) \\ &= \boldsymbol{w} - \lambda \left(\frac{\partial \ell_{\text{logistic}}(z)}{\partial z}\Big|_{z=y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n \boldsymbol{x}_n \\ &= \boldsymbol{w} - \lambda \left(\frac{-e^{-z}}{1+e^{-z}}\Big|_{z=y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n \boldsymbol{x}_n \\ &= \boldsymbol{w} + \lambda\, \sigma(-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) y_n \boldsymbol{x}_n \\ &= \boldsymbol{w} + \lambda\, \mathbb{P}(-y_n \mid \boldsymbol{x}_n; \boldsymbol{w}) y_n \boldsymbol{x}_n\end{aligned}$$

This is a *soft version of Perceptron!*

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



Newton method

Newton's method is an extension of steepest descent, where the second-order term in the Taylor series is used.

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2$$

Let us minimize the right hand side:

$$f'(x_0) + f''(x_0)(x - x_0) = 0 \quad \text{or} \quad x = x_0 - \frac{f'(x_0)}{f''(x_0)}$$

We will literate this procedure

$$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$$

Deriving Newton method

This could be generalized for functions f of several variables:

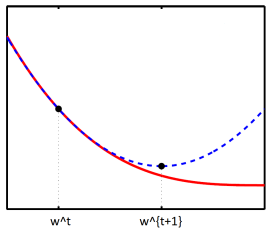
$$x_{n+1} = x_n - \boldsymbol{H}^{-1}(x_n)\, \nabla f(x_n)$$

where $\boldsymbol{H}$ is the Hessian

$$H_{ij} = \frac{\partial^2 F(\boldsymbol{x})}{\partial x_i \partial x_j}$$

Therefore, for convex F (so H_t is *positive semidefinite*) we obtain **Newton method**:

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \boldsymbol{H}_t^{-1} \nabla F(\boldsymbol{w}^{(t)})$$



Comparing GD and Newton

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \lambda \nabla F(\boldsymbol{w}^{(t)}) \qquad \text{(GD)}$$
$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \boldsymbol{H}_t^{-1} \nabla F(\boldsymbol{w}^{(t)}) \qquad \text{(Newton)}$$

Both are iterative optimization procedures, but Newton method

- has no learning rate λ (*so no tuning needed!*)
- converges *super fast* in terms of #iterations needed
- requires **second-order** information

Applying Newton to logistic loss

$$\nabla_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) = -\sigma(-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) y_n \boldsymbol{x}_n$$

$$\begin{aligned}
\nabla^2_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) &= \left(\frac{\partial \sigma(z)}{\partial z}\Big|_{z=-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n^2 \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}} \\
&= \left(\frac{e^{-z}}{(1+e^{-z})^2}\Big|_{z=-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}} \\
&= \sigma(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) \left(1 - \sigma(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)\right) \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}}
\end{aligned}$$

Exercises:

- why is the Hessian of logistic loss positive semidefinite?
- can we apply Newton method to perceptron/hinge loss?

Outline

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 $f : \mathbb{R}^{\mathsf{D}} \to [\mathsf{C}]$

Examples:

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

Nearest Neighbor Classifier naturally works for arbitrary C.

Linear models: from binary to multiclass

What should a linear model look like for multiclass tasks?

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

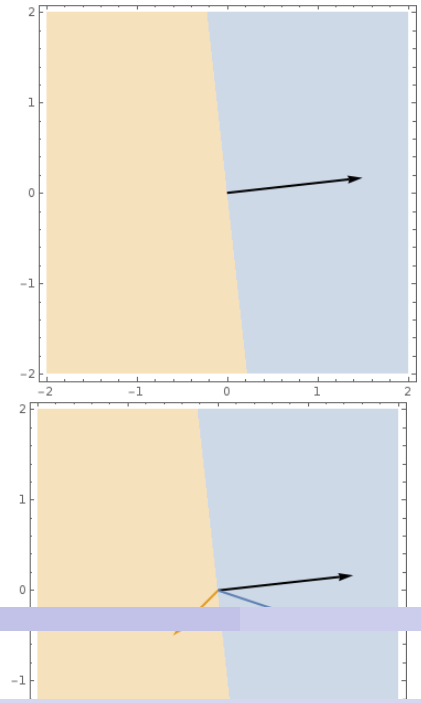
$$f(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \geq 0 \\ 2 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} < 0 \end{cases}$$

By setting $\boldsymbol{w} = \boldsymbol{w}_1 - \boldsymbol{w}_2$, it can be written as

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

for any $\boldsymbol{w}_1, \boldsymbol{w}_2$.
Think of $\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}$ as **a score for class** k.

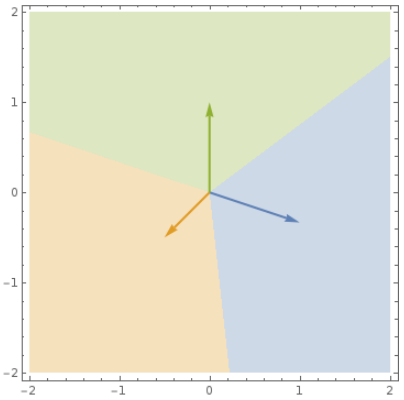
Linear models: from binary to multiclass



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

- Blue class:
  $\{\boldsymbol{x} : \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} > 0\}$
  $\{\boldsymbol{x} : 1 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}\}$
- Orange class:

Linear models: from binary to multiclass



$\boldsymbol{w}_1 = (1, -\frac{1}{3})$
$\boldsymbol{w}_2 = (-\frac{1}{2}, -\frac{1}{2})$
$\boldsymbol{w}_3 = (0, 1)$

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

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

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

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

Naturally, for class $y = y_n$

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

This is called the *softmax function*.

Applying MLE again

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

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

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

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

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

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

Optimization

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

$$g(\boldsymbol{W}) = \ln \left(1 + \sum_{k \neq y_n} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n} \right) ?$$

This is a $\mathsf{C} \times \mathsf{D}$ matrix.

Take the derivative wrt $\boldsymbol{w}_j \neq \boldsymbol{w}_{y_n}$:

$$\begin{aligned}
\nabla_{\boldsymbol{w}_j} g(\boldsymbol{W}) &= \frac{e^{(\boldsymbol{w}_j - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n}}{1 + \sum_{k \neq y_n} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}} \\
&= \frac{e^{\boldsymbol{w}_j^{\mathrm{T}}\boldsymbol{x}_n}}{e^{\boldsymbol{w}_{y_n}^{\mathrm{T}}\boldsymbol{x}_n} + \sum_{k \neq y_n} e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}} \\
&= \frac{e^{\boldsymbol{w}_j^{\mathrm{T}}\boldsymbol{x}_n}}{\sum_{k \in [\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}} = \mathbb{P}(j \mid \boldsymbol{x}_n; \boldsymbol{W}) \boldsymbol{x}_n^{\mathrm{T}}
\end{aligned}$$

Optimization

Apply **SGD**

$$g(\boldsymbol{W}) = \ln \left(1 + \sum_{k \neq y_n} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n} \right)$$

Take the derivative wrt $\boldsymbol{w}_{y_n}$.

$$\begin{aligned}
\nabla_{\boldsymbol{w}_{y_n}} g(\boldsymbol{W}) &= -\frac{\sum_{k \neq y_n} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n}}{1 + \sum_{k \neq y_n} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}} \\
&= -1 + \frac{1}{1 + \sum_{k \neq y_n} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}} \\
&= -1 + \frac{e^{\boldsymbol{w}_{y_n}^{\mathrm{T}}\boldsymbol{x}_n}}{\sum_{k \in [\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}_n}} \boldsymbol{x}_n^{\mathrm{T}} = \left(-1 + \mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{W})\right) \boldsymbol{x}_n^{\mathrm{T}}
\end{aligned}$$

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

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

Think about why the algorithm makes sense.

Consider $\mathbb{P}(y = y_n) \to 1$ and $\mathbb{P}(y = y_n) \to 0$...

A note on prediction

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

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

In either case, **mistake is bounded by logistic loss**.

- deterministic

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

  Indeed, there is such k that $\boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x} \geq \boldsymbol{w}_y^{\mathrm{T}} \boldsymbol{x}$, therefore the argument of $\log$ is larger than 2.

A note on prediction

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

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

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

- randomized

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

Here we used the fact that $1 - z \leq -\ln z$,
which follows form the Taylor expansion: $\ln(1 + x) = x + O(x^2)$.

Reduce multiclass to binary

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

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.

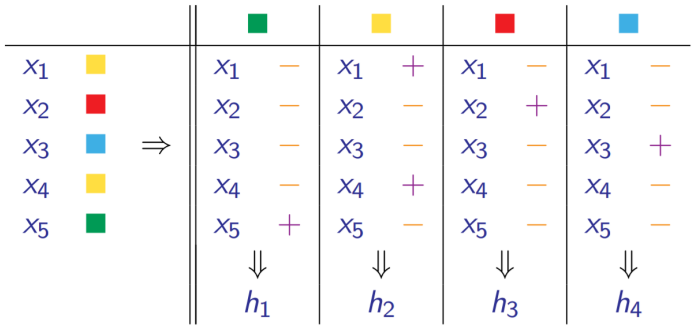
- **one-versus-all** (one-versus-rest, one-against-all, etc)
- **one-versus-one** (all-versus-all, etc)
- **Error-Correcting Output Codes** (ECOC)
- **tree-based reduction**

One-versus-all (OvA)

Idea: make C binary classifiers.

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

- relabel each example with class k as $+1$, and all others as -1
- train a binary classifier h_k using this new dataset (what size?)



One-versus-all (OvA)

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

- ask each h_k: **does this belong to class k?** (i.e. $h_k(\boldsymbol{x})$)
- could be several h_k s.t. $h_k(\boldsymbol{x}) = +1$.
- randomly pick one

OvA becomes inefficient as the number of classes rises.

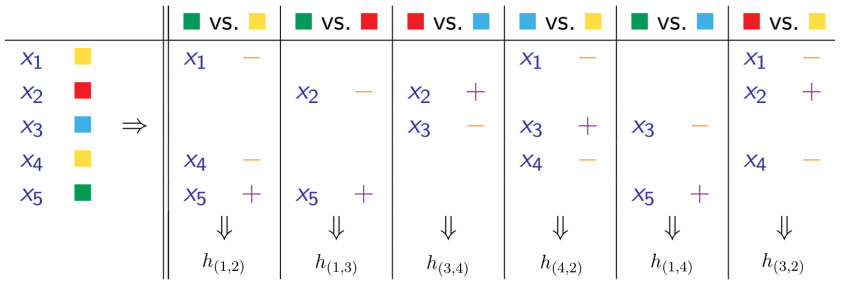
It's possible to create a significantly more efficient OvA model with a deep neural network.

One-versus-one (OvO)

Idea: make $\binom{\mathsf{C}}{2}$ binary classifiers.

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

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



One-versus-one (OvO)

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

- ask each classifier $h_{(k,k')}$ to **vote for either class k or k'**
- predict the class with the most votes (break tie in some way)

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

Error-correcting output codes (ECOC)

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 on each column of $\boldsymbol{M}$.

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 ■	⇒	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 +
		⇓	⇓	⇓	⇓	⇓
		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** $\boldsymbol{c} = (h_1(\boldsymbol{x}), \ldots, h_{\mathsf{L}}(\boldsymbol{x}))^{\mathrm{T}}$
- predict the class with the **most similar code**: $k = \operatorname{argmax}_k (\boldsymbol{M}\boldsymbol{c})_k$

Suppose you have two classes

- 1: {+,-,-,-,-}
- 2: {-,+,+,+,+}

and the predicting code is {+,+,+,-,-}. Which class does it predict?

Class 1, since it makes only 2 mistakes.

Error-correcting output codes (ECOC)

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

- the more *dissimilar* the codes between different classes are, the better
- *random code* is a good choice, but might create *hard* training sets

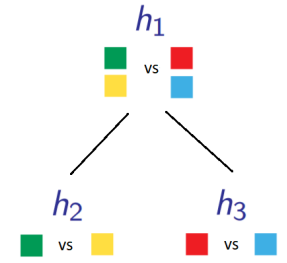
One-versus-all ($L = \mathsf{C}$) and One-versus-one ($L = \binom{\mathsf{C}}{2}$) are two examples of ECOC.

Tree based method

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

Training: see pictures. In the tree each leaf is a single class.

		■ vs ■	■ vs ■	■ vs ■
x_1 ■		x_1 +	x_1 −	
x_2 ■		x_2 −		x_2 +
x_3 ■	⇒	x_3 −		x_3 −
x_4 ■		x_4 +	x_4 −	
x_5 ■		x_5 +	x_5 +	
		⇓	⇓	⇓
		h_1	h_2	h_3



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

Comparisons

In big-O notation,

Reduction	**test time**	**#training points**	**remark**
OvA	C	CN	not robust
OvO	C^2	CN	can achieve very small training error
ECOC	L	LN	need diversity when designing code
Tree	$\log_2 C$	$(\log_2 C)N$	good for "extreme classification"

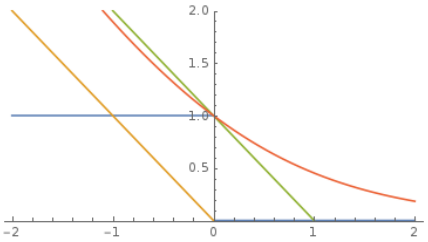
Summary

Linear models for classification:

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

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

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):

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

using **GD/SGD/Newton**.