CSCI567 Machine Learning (Fall 2024)

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September 13, 2024

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

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This lecture: **binary classification**

- Number of classes: $\mathsf{C} = 2$
- Labels: $\{-1, +1\}$ (cat or dog, fraud or not, price up or down...)

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We have discussed **nearest neighbor classifier**:

- require carrying the training set
- more like a heuristic

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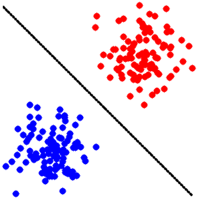

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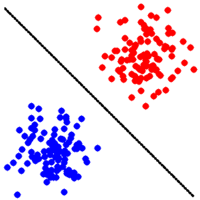
Sign of $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ predicts the label:

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

(Sometimes use sgn for sign too.)



The models

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

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

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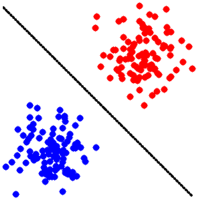
for all $n \in [N]$.



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

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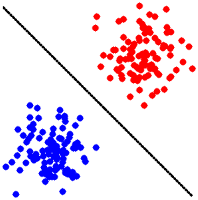
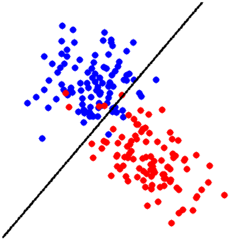


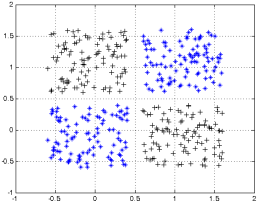
The models

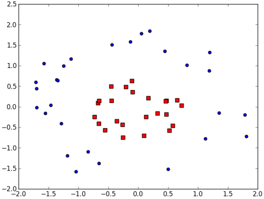
Still makes sense for “almost” linearly separable data



The models

For clearly not linearly separable data,





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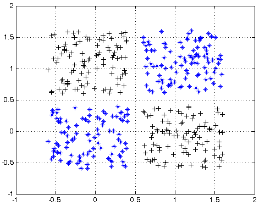

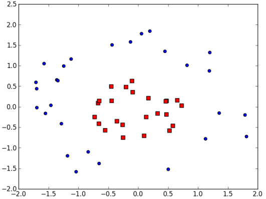

Again can apply a **nonlinear mapping** $\mathbf{\Phi}$:

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

More discussions in the next two lectures.

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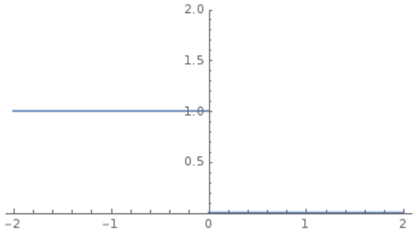
For classification, more convenient to look at the loss **as a function of** $y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$. That is, with

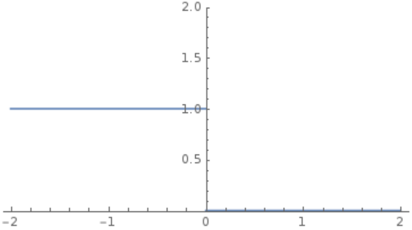
$$\ell_{\text{0-1}}(z) = \mathbb{I}[z \leq 0]$$



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

Minimizing 0-1 loss is hard

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



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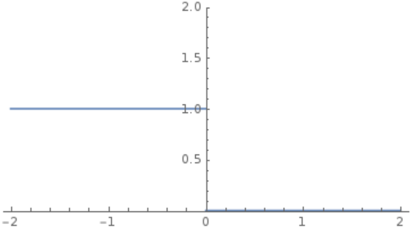
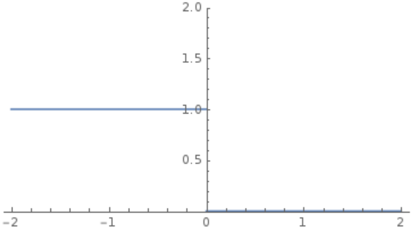


Even worse, minimizing 0-1 loss is *NP-hard in general*.

Surrogate Losses

Solution: find a **convex surrogate loss**



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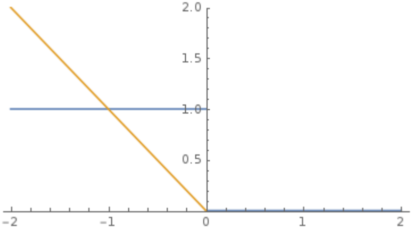

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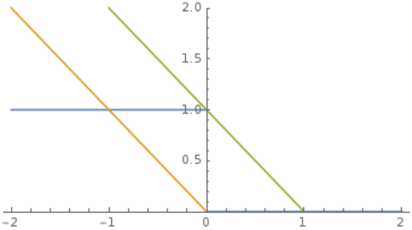

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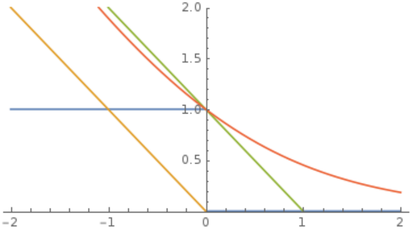

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- hinge loss $\ell_{\text{hinge}}(z) = \max\{0, 1 - z\}$(used in SVM and many others)
- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$ (used in logistic regression; the base of $\log$ doesn't matter)

ML becomes convex optimization

Step 3. Find ERM:

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

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

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Note: minimizing perceptron loss *does not really make sense* (try $\boldsymbol{w} = \mathbf{0}$), but the algorithm derived from this perspective does.

Outline

A simple view

In one sentence: find the minimizer of

$$F(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N} \ell_{\mathsf{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$
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Before optimizing it: *why logistic loss? and why "regression"?*

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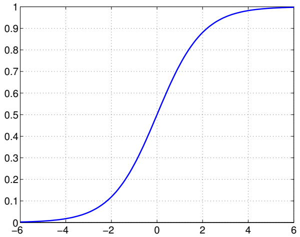
One way: **sigmoid function + linear model**

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

where σ is the sigmoid function:

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



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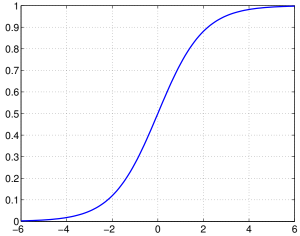

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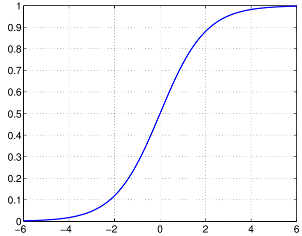

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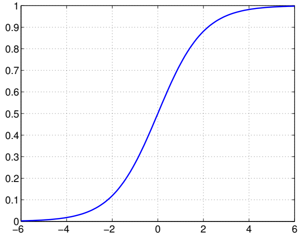

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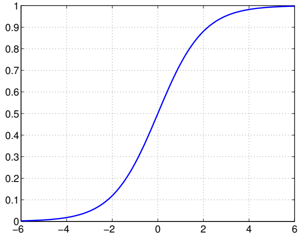

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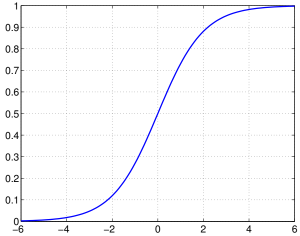

The probability of label -1 is naturally

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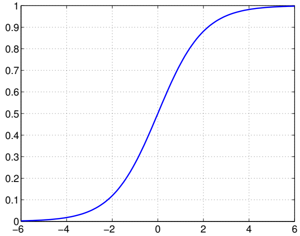

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and thus

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

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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

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

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&= \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

$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \tilde{\nabla} F(\boldsymbol{w})$$

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\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.})
\end{aligned}
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Let's apply SGD again

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\begin{aligned}
\boldsymbol{w} &\leftarrow \boldsymbol{w} - \eta \tilde{\nabla} F(\boldsymbol{w}) \\
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&= \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
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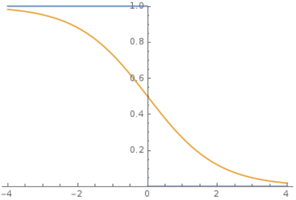
\end{aligned}
$$

This is a *soft version of Perceptron!*

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



Applying Newton to logistic loss

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

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Exercises:

- why is the Hessian of logistic loss positive semidefinite?

Applying Newton to logistic loss

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Exercises:

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

Outline

Recall the perceptron loss

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

Let's approximately minimize it with GD/SGD.

Applying GD to perceptron loss

Objective

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

Applying GD to perceptron loss

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

Gradient (or really *sub-gradient*) is

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

(only misclassified examples contribute to the gradient)

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GD update

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Slow: each update makes one pass of the entire training set!

Applying SGD to perceptron loss

How to construct a stochastic gradient?

Applying SGD to perceptron loss

How to construct a stochastic gradient?

One common trick: pick one example $n \in [N]$ uniformly at random, let

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

clearly unbiased (convince yourself).

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Fast: each update touches only one data point!

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Conveniently, objective of most ML tasks is a *finite sum* (over each training point) and the above trick applies!

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

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Note:

- $\boldsymbol{w}$ is always a *linear combination* of the training examples
- why $\eta = 1$? Does not really matter in terms of prediction of $\boldsymbol{w}$

Why does it make sense?

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

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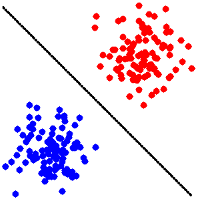
Thus it is more likely to get it right after the update.

Any theory?

(HW 1) If training set is linearly separable

- Perceptron *converges in a finite number of steps*
- training error is 0



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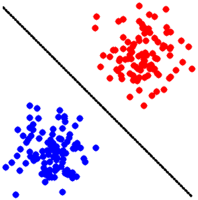

There are also guarantees when the data are not linearly separable.