CSCI567 Machine Learning (Spring 2021)

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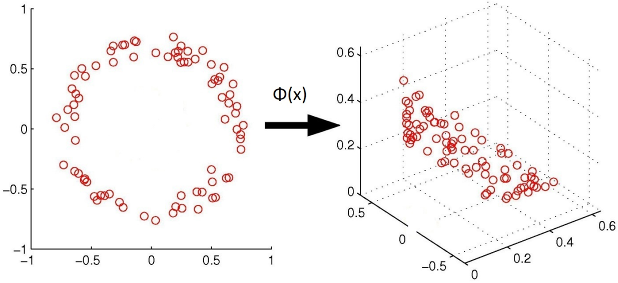
Outline

1. Review of Last Lecture
2. Linear Classifier and Surrogate Losses
3. Perceptron

Outline

Regression with nonlinear basis



Model: $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$ where $\boldsymbol{w} \in \mathbb{R}^M$

Similar least square solution: $\boldsymbol{w}^* = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$

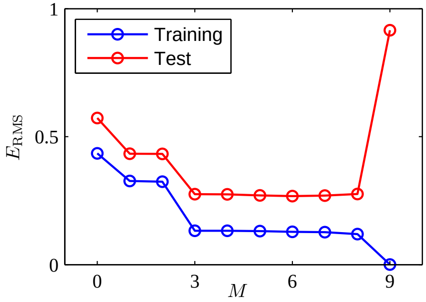
Underfitting and Overfitting

$M \leq 2$ is *underfitting* the data

- large training error
- large test error

$M \geq 9$ is *overfitting* the data

- small training error
- **large test error**



How to prevent overfitting? more data + regularization

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}} \left(\mathrm{RSS}(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_2^2\right) = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{y}$$

General idea to derive ML algorithms

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

- e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$
- e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\Phi}(\boldsymbol{x}) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{M}}\}$

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

Step 3. Find **empirical risk minimizer (ERM)**:

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

or **regularized empirical risk minimizer**:

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

ML becomes optimization

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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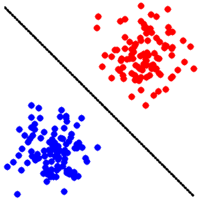

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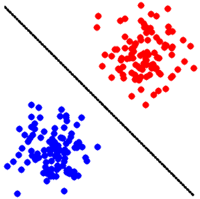
Sign of $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ predicts the label:

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

(Sometimes use sgn for sign too.)



The models

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

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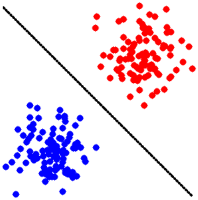
Good choice for *linearly separable* data, i.e., $\exists \boldsymbol{w}$ s.t.

$$\mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x_n}) = y_n$$

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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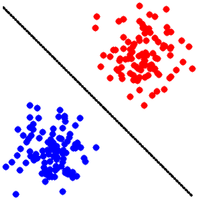
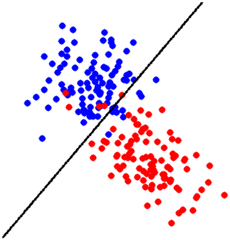


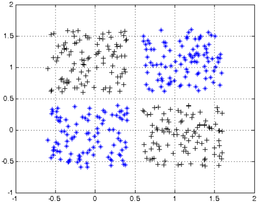
The models

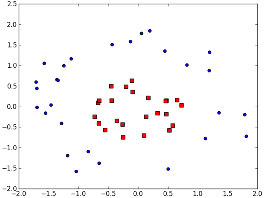
Still makes sense for “almost” linearly separable data



The models

For clearly not linearly separable data,





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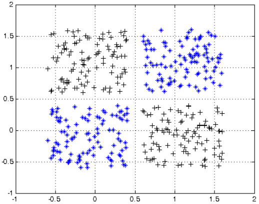

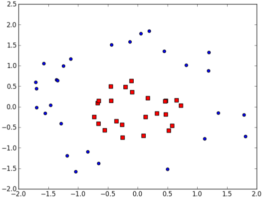

Again can apply a **nonlinear mapping** $\boldsymbol{\Phi}$:

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

More discussions in the next two lectures.

0-1 Loss

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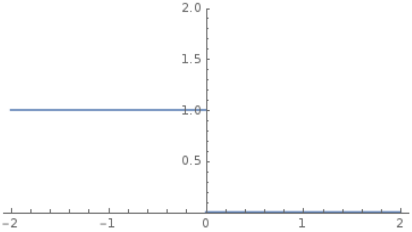
For classification, more convenient to look at the loss **as a function of** $\boldsymbol{y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}}$ (see ESL 4.5). That is, with

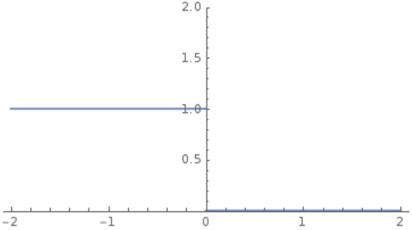
$$\ell_{\text{0-1}}(z) = \mathbb{I}[z \leq 0]$$



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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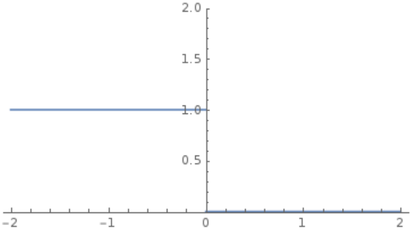
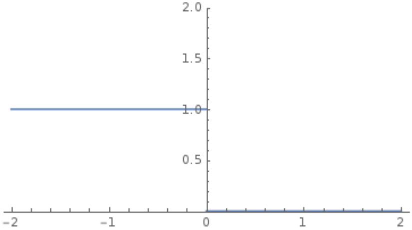


Even worse, minimizing 0-1 loss is *NP-hard in general*.

Surrogate Losses

Solution: find a **convex surrogate loss**



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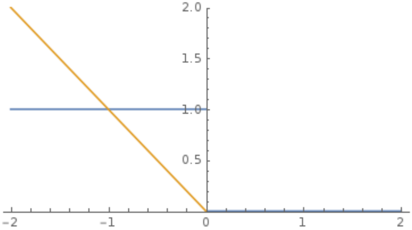

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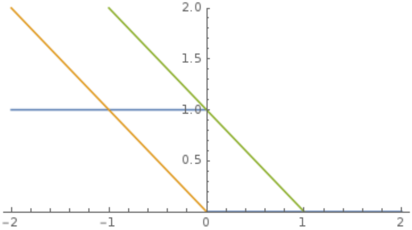

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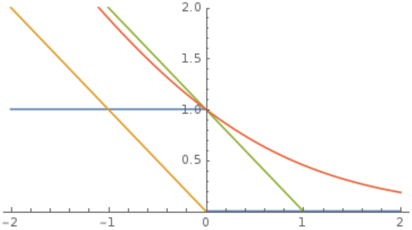

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- hinge loss $\ell_{\text{hinge}}(z) = \max\{0, 1-z\}$(used in SVM and many others)
- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$ (used in logistic regression; the base of $\log$ doesn't matter)

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.

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The Perceptron Algorithm

In one sentence: Stochastic Gradient Descent applied to perceptron loss

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i.e. find the minimizer of

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

using SGD

A detour of numerical optimization methods

We describe two simple yet extremely popular methods

- **Gradient Descent (GD)**: simple and fundamental
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Gradient is sometimes referred to as *first-order* information of a function. Therefore, these methods are called *first-order methods*.

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Start from some $\boldsymbol{w}^{(0)}$. For $t = 0, 1, 2, \ldots$

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

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- in theory η should be set in terms of some parameters of F
- in practice we just try several small values

An example

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

Why GD?

Intuition: by first-order **Taylor approximation**

$$F(\boldsymbol{w}) \approx F(\boldsymbol{w}^{(t)}) + \nabla F(\boldsymbol{w}^{(t)})^{\mathrm{T}}(\boldsymbol{w} - \boldsymbol{w}^{(t)})$$

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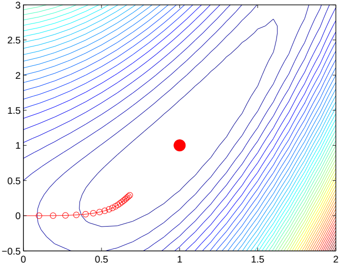

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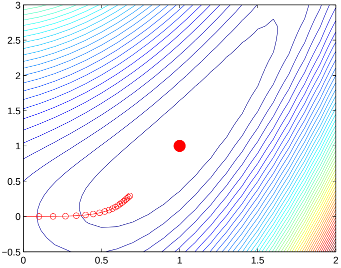

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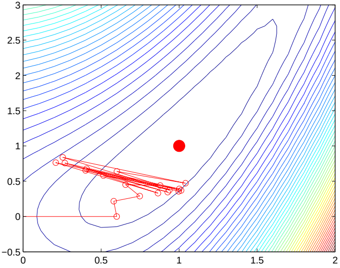

but large η is unstable

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where $\tilde{\nabla} F(\boldsymbol{w}^{(t)})$ is a random variable (called **stochastic gradient**) s.t.

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

Convergence Guarantees

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Even for *nonconvex objectives*, many recent works show effectiveness of GD/SGD.

Applying GD to perceptron loss

Objective

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GD update

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

Applying GD to perceptron loss

Objective

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

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)

GD update

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

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

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clearly unbiased (convince yourself).

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Exercise: try SGD to minimize RSS for linear regression.

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Note:

- $\boldsymbol{w}$ is always a *linear combination* of the training examples

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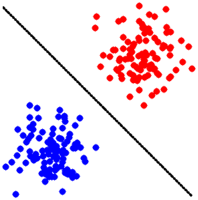
Thus it is more likely to get it right after the update.

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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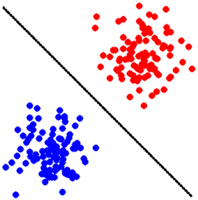

There are also guarantees when the data are not linearly separable.