Linear Classification

Machine Learning

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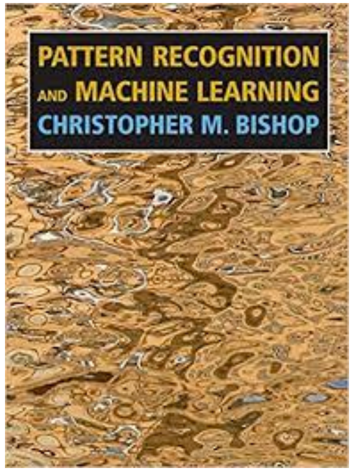
POLITECNICO
MILANO 1863

References

- *Pattern Recognition and Machine Learning*, Bishop
  - Chapter 4 (4.1.1 - 4.1.3, 4.1.7, 4.3.1, 4.3.2)



Outline

- ❑ Linear Classification Models

- ❑ Direct Approaches
  - ▶ Least Squares for Classification
  - ▶ The Perceptron Algorithm

- ❑ Probabilistic Discriminative Approach
  - ▶ Logistic Regression

A quick recap

What is classification?

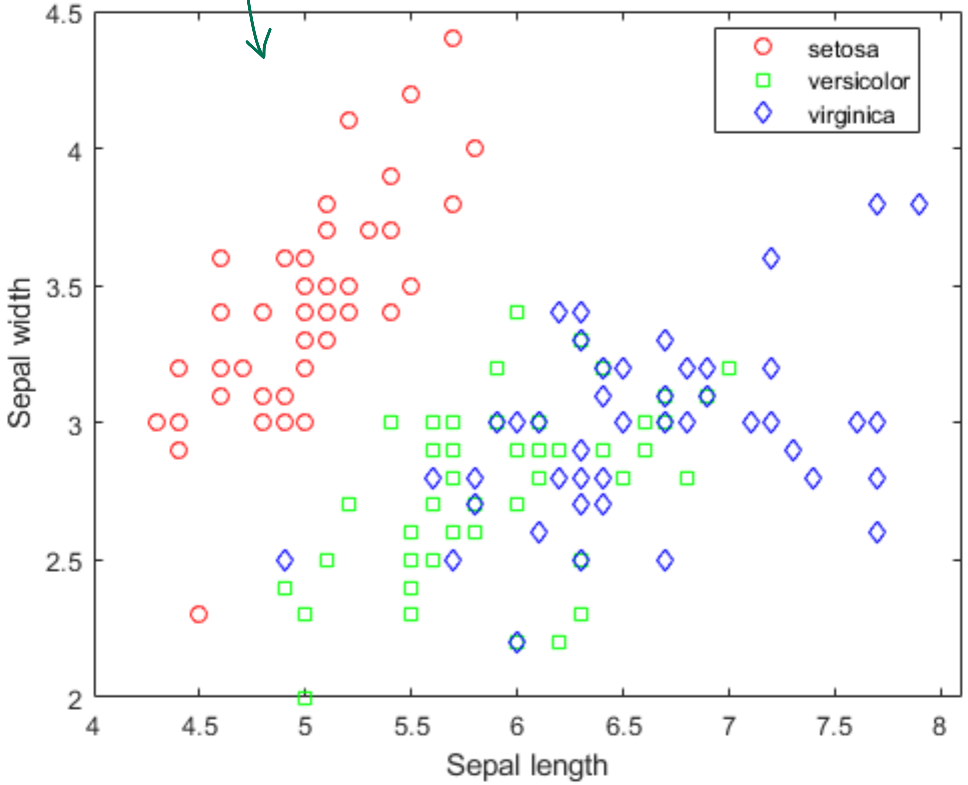
- ❑ Learn, from a dataset $\mathcal{D}$, an **approximation** of function $f(x)$ that maps input x to a discrete class C_k (with $\mathrm{k} = 1, \dots, K$)

$$\mathcal{D} = \{\langle x, C_k \rangle\} \Rightarrow C_k = f(x)$$

  - How do we model f?
  - How do we encode C_k?
  - How do we evaluate our approximation?
  - How do we optimize our approximation?

$\left.\begin{array}{l}\text{How do we model } f?\\ \text{How do we encode } C_k?\end{array}\right)$ Model

3 classes problem



Classification approaches

- Discriminant function
  - Model a parametric function that maps input to classes
  - Learn parameters from data
- Probablistic discriminative approach
  - Design a parametric model of $p(C_k|\mathbf{x})$
  - Learn model parameters from data
- Probabilistic generative approach
  - Model $p(\mathbf{x}|C_k)$ and class priors $p(C_k)$
  - Fit models to data
  - Infer **posterior** with Bayes’ rule: $p(C_k|\mathbf{x}) = p(\mathbf{x}|C_k)p(C_k)/p(\mathbf{x})$

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Discriminant Function

Generalized Linear Models for classification

- In linear classification, we will use $\overbrace{\textbf{generalized linear models}}^{\text{GLM}}$:

$$f(\mathbf{x},\mathbf{w}) = f\left(w_0 + \sum_{j=1}^{D-1} w_j x_j\right) = f(\underbrace{\mathbf{x}^T\mathbf{w} + w_0}_{\text{our model in linear regression.}})$$

f(linear model)

  - f(·) is **not** linear in $\mathbf{w}$ due to the (non linear) **activation function** f, because its output is either a discrete label or a probability value
  - f(·) partitions the input space into **decision regions** whose boundaries are called **decision boundaries** or **decision surfaces**
  - these decision surfaces are linear function of $\mathbf{x}$ and $\mathbf{w}$, as they correspond to $\mathbf{x}^T\mathbf{w} + w_0 = \text{const}$

    That's why "GLM"
  - generalized linear models are more complex to use with respect to linear models (both from a computational and analytical perspective)

Label Encoding

K=2 classes

- ❑ A common encoding for two-class problems is a binary encoding: $t \in \{0,1\}$
  - $t = 1$ encodes **positive** class and $t = 0$ encodes **negative** one
  - with this encoding, t and $\mathrm{f}(\cdot)$ represent the **probability** of positive class
- ❑ A possible alternative encoding for two-class problems is $t \in \{-1,1\}$
  - this encoding is convenient for some algorithms

"Binary problem"

K classes

- ❑ When the problem has K classes, a typical choice is **1-of-K** encoding
  - t is a vector of length K, with a 1 in the position corresponding to the encoded class
  - with this encoding, t and $\mathrm{f}(\cdot)$ represent the probability density over the classes
  - as an example, a data sample that belongs to class 4 of a problem with K=5, is encoded as $t = (0,0,0,1,0)^T$

"Multiclass problem"

or "ONE HOT ENCODING".

Discriminant linear function for a two-class problem

Binary classification

$$f(\mathbf{x},\mathbf{w}) = \begin{cases} C_1, & \text{if } \overbrace{\mathbf{x}^T\mathbf{w} + w_0}^{y(\mathbf{x})} \geq 0 \\ C_2, & \text{otherwise} \end{cases}$$

encoded either via {0,1} or via {-1,1}.

we use a slightly different notation compared to lin. reg.: w_0 is not included in w.

Reason: for some properties we need to see explicitly w_0.

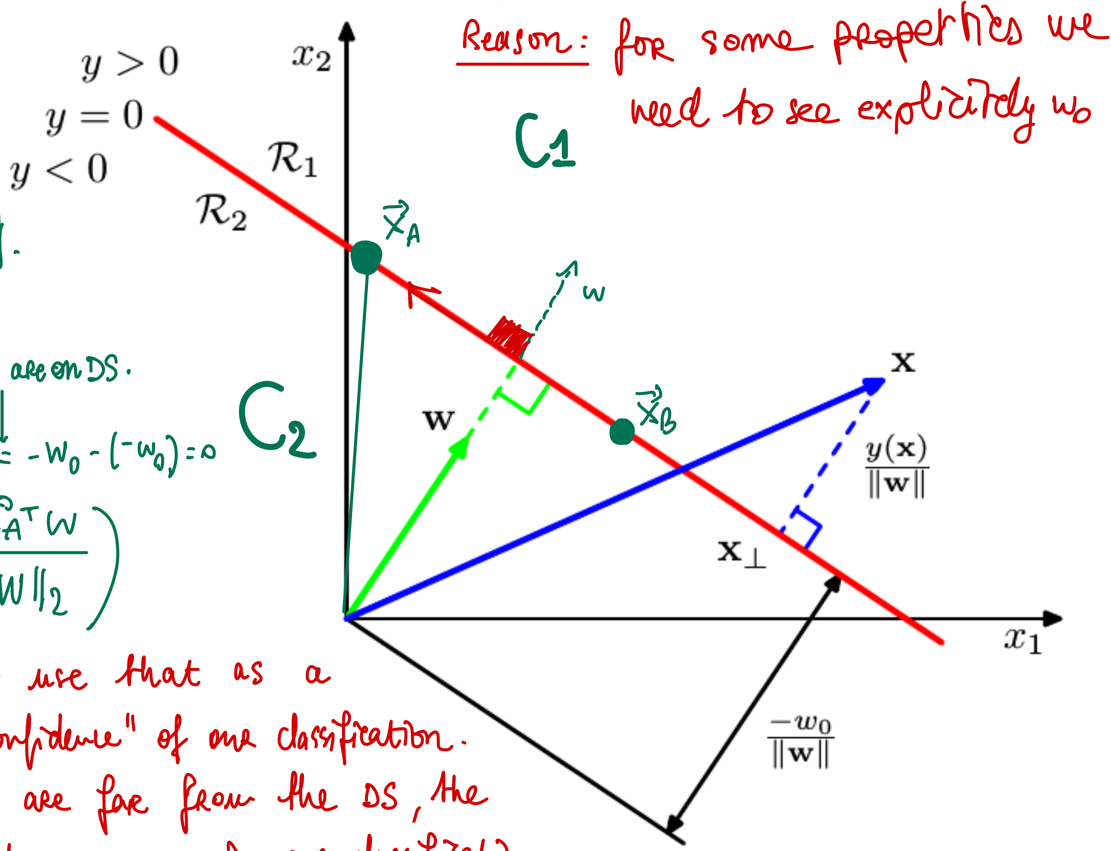
❑ Properties

- DS is $y(\cdot) = \mathbf{x}^T\mathbf{w} + w_0 = 0$
- DS is orthogonal to $\mathbf{w}$: $(\vec{x}_A - \vec{x}_B)\cdot w = \vec{x}_A w - \vec{x}_B w \overset{\text{A\&B are on DS.}}{=} -w_0 - (-w_0) = 0$
- distance of DS from origin is $-\frac{w_0}{\|\mathbf{w}\|_2} \left(= \frac{\vec{x}_A^T w}{\|w\|_2} \right)$
- "distance" of $\mathbf{x}$ from DS is $\frac{y(\mathbf{X})}{\|\mathbf{W}\|_2}$

" " because it has a sign.

NB: We can use that as a measure of "confidence" of our classification. The more we are far from the DS, the more confident we are in our classification.
↳ cf later is SVM.

DS: "Decision Surface" or "Decision Boundary"



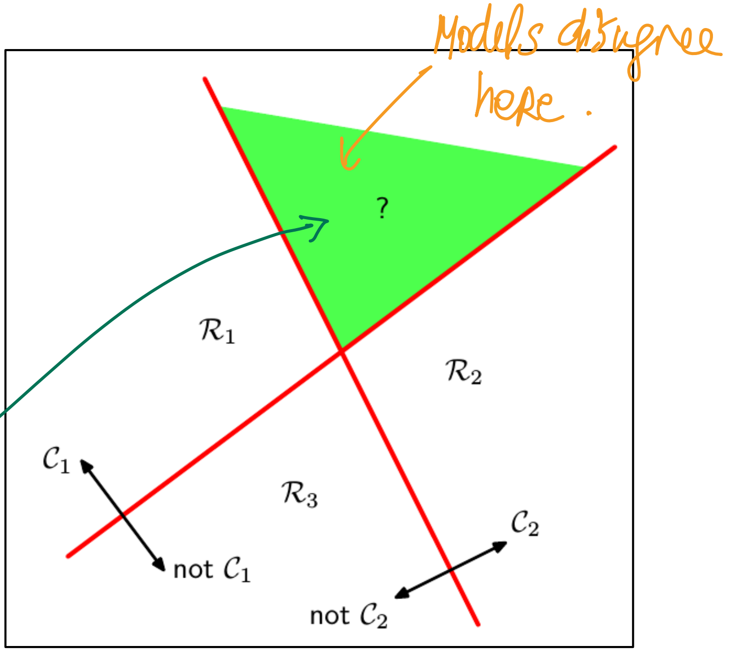
Now, our question is: HOW TO LEARN W ?

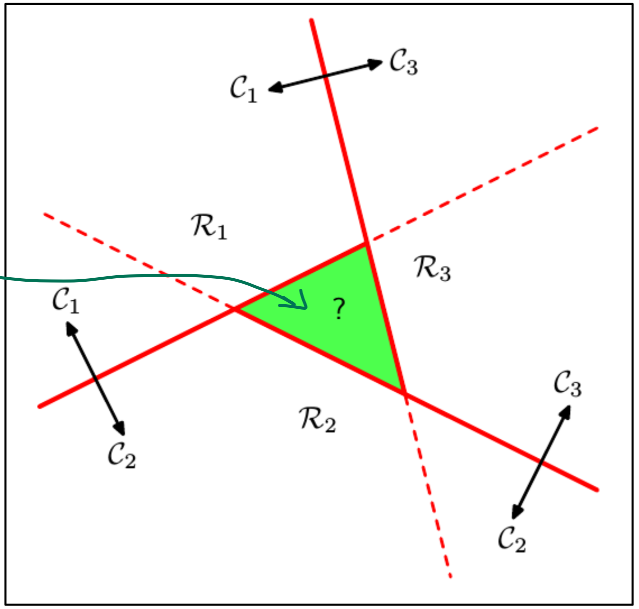
How to deal with multiple classes problems?

- ❑ In a multi-class problem we have K classes
- ❑ **One-versus-the-rest** approach uses K-1 **binary cassifiers** (i.e., that solve a two-class problem)
  - each classifier discriminates C_i and $\text{not}\ C_i$ regions
  - **ambiguity:** region mapped to several classes
- ❑ **One-versus-one** approach uses K(K-1)/2 class binary classifiers
  - each classifier discriminates between C_i and C_j
  - similary ambiguity of previous approach

2 main methods

HOW TO SOLVE THIS ISSUE OF AMBIGUITY?





A simple solution for multiple classes

I choose the class in which the model is the most confident.

- ❑ A possible solutions is to use K linear discriminant functions:

$$y_k(\mathbf{x}) = \mathbf{x}^T \mathbf{w}_k + w_{k0}, \text{ where } k = 1, \ldots, K$$

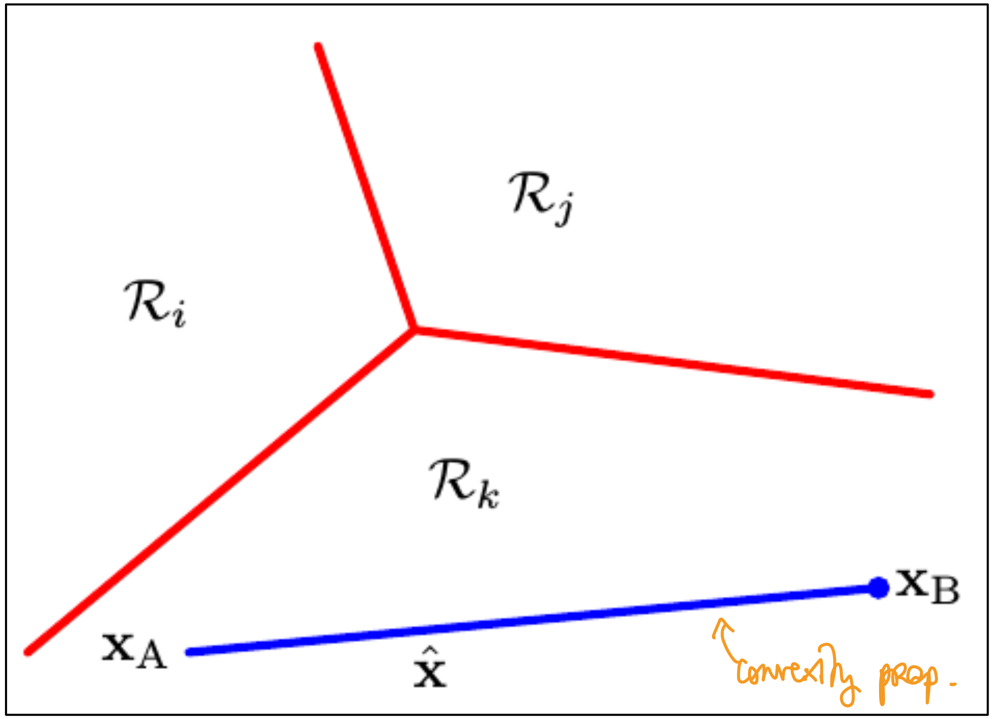
- Map $\mathbf{x}$ to class C_k if $y_k > y_j \quad \forall j \neq k$
- No ambiguity !!
- DS are **singly connected** and **convex**

Let $\mathbf{x}_A, \mathbf{x}_b \in \mathcal{R}_k$

Thus, $y_k(\mathbf{x}_A) > y_j(\mathbf{x}_A)$ and $y_k(\mathbf{x}_B) > y_j(\mathbf{x}_B)$

$\Rightarrow \forall \alpha \; (0 < \alpha < 1)$

$y_k(\alpha \mathbf{x}_A + (1-\alpha)\mathbf{x}_B) > y_j(\alpha \mathbf{x}_A + (1-\alpha)\mathbf{x}_B)$



HOW TO FIND W ?

1st method

Least Squares for Classification

It's possible but it has some problems.

- ❑ Let consider a K-class problem and use a $\overbrace{\text{1-of-K}}^{\text{1 hot encoding}}$ encoding for target
- ❑ Each class is modeled with a linear function:

$$y_k(\mathbf{x}) = \mathbf{x}^T \mathbf{w}_k + w_{k0}, \text{ where } k = 1, \ldots, K$$

- ❑ In matrix notation:

$$\mathbf{y}(\mathbf{x}) = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}$$

  - ▶ $\widetilde{\mathrm{W}}$ has size (D+1)xK
  - ▶ k-th column of $\widetilde{\mathrm{W}}$ is $\widetilde{\mathbf{w}_{\boldsymbol{k}}} = \left(w_{k0}, \mathbf{w}_k^T\right)^T$
  - ▶ $\tilde{\mathbf{x}} = (1, \mathbf{x}^T)^T$

1st method

Least Squares for Classification (2)

It's possible but it has some problems.

- ❑ Given a dataset $\mathcal{D} = \{\mathbf{x}_i, \mathbf{t}_i\}$, where i=1,...,N
- ❑ We can apply Least Squares to find the optimal value of $\widetilde{\mathbf{W}}$

$$\tilde{\mathbf{W}} = \left(\tilde{\mathbf{X}}^T\tilde{\mathbf{X}}\right)^{-1}\tilde{\mathbf{X}}^T\mathbf{T}$$

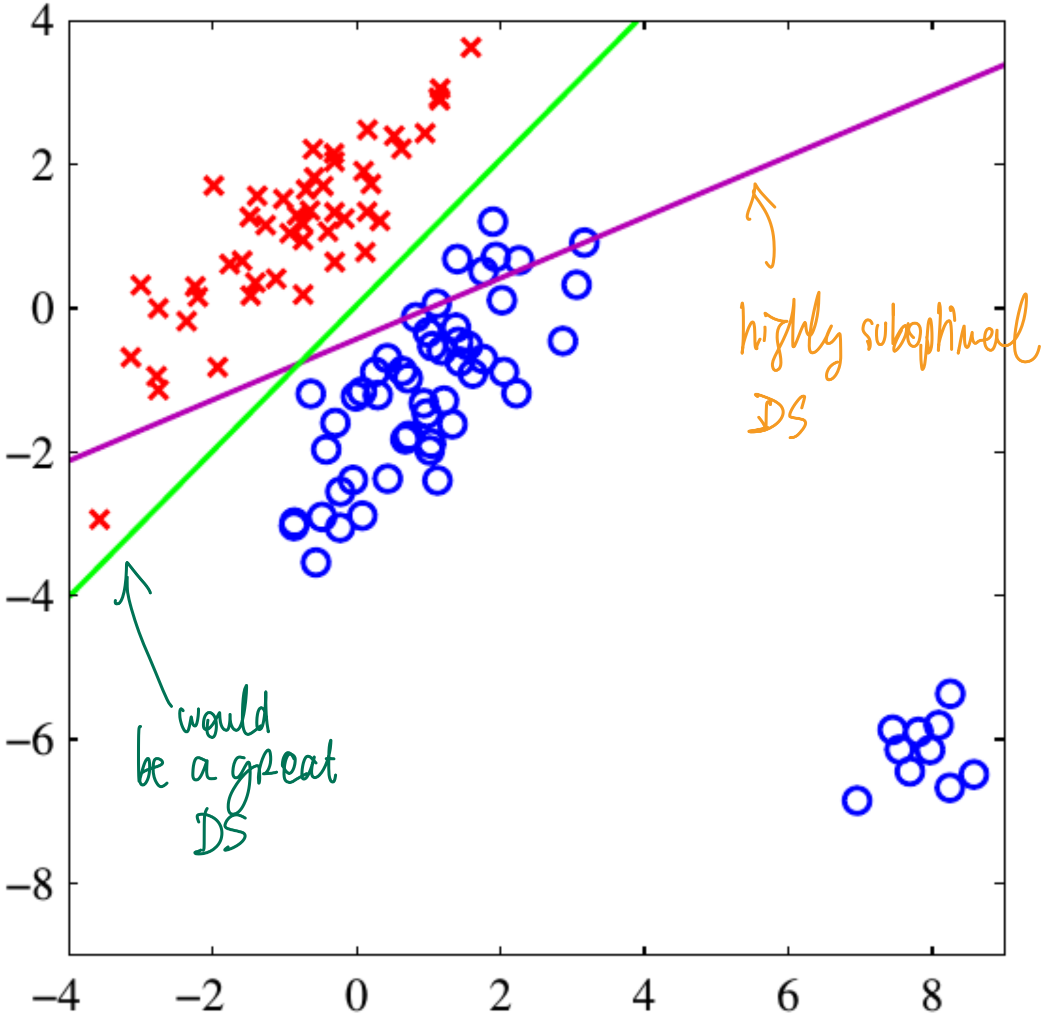
  - ▸ $\tilde{\mathbf{X}}$ is a Nx(D+1) matrix whose i-th is $\tilde{\mathbf{x}}_i^T$
  - ▸ $\mathbf{T}$ is a NxK matrix whose i-th row is $\mathbf{t}_i^T$

- ❑ Any new sample $\tilde{\mathbf{x}}_{new}^T$ is mapped to class C_k if $t_k > t_j \quad \forall j$, where t_k is the k-th component of the model output, computed as $t_k = \tilde{\mathbf{x}}^T\widetilde{\mathbf{w}_k}$

1st method

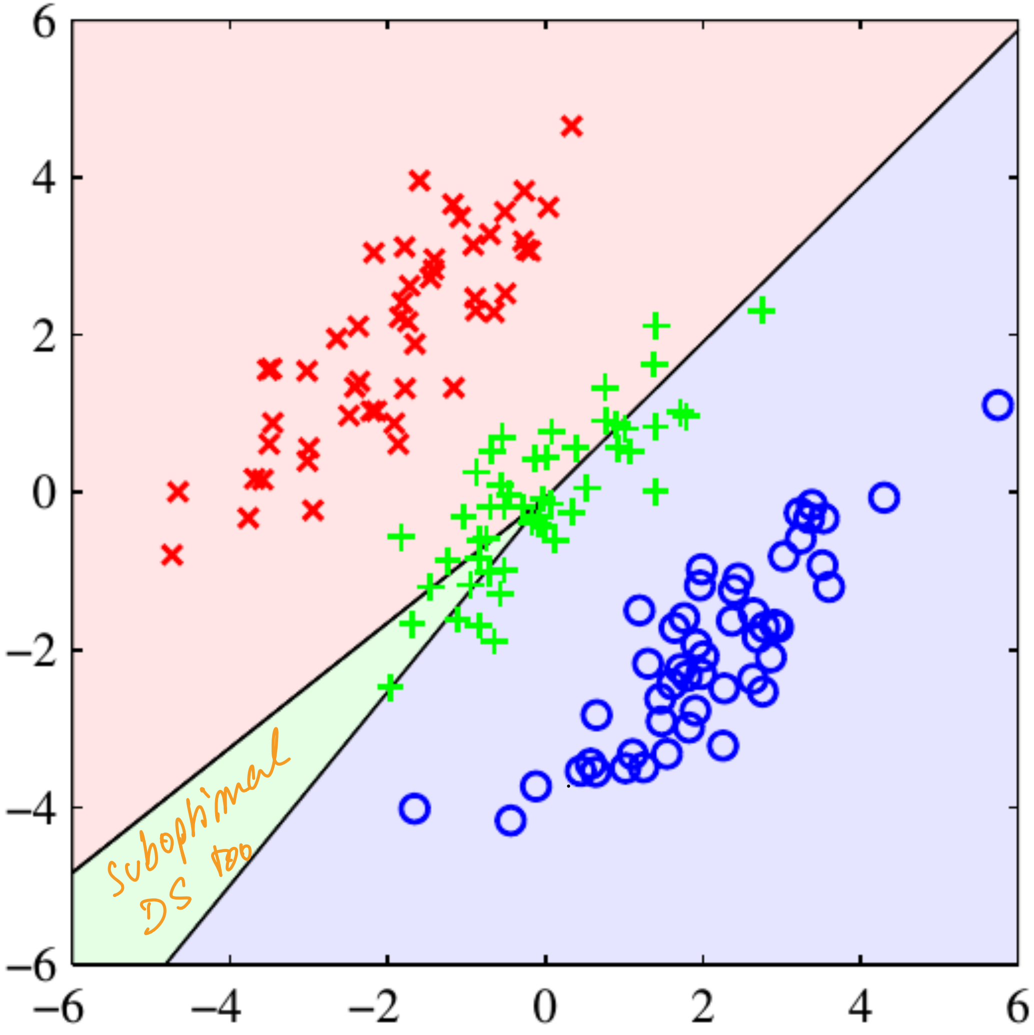
Problems with Least Squares: Outliers and Output Distribution

→ OLS is **NOT** a good approach for classification problem !



highly suboptimal DS

would be a great DS



suboptimal DS too

WHAT IS THEN A GOOD SOLUTION ?

Parenthesi

Linear Basis Function Models

- □ So far we considered models that work in the **input space** (i.e., with $\mathbf{x}$)
- □ However, we can still extend models by using a fixed set of basis function $\phi(\mathbf{x})$

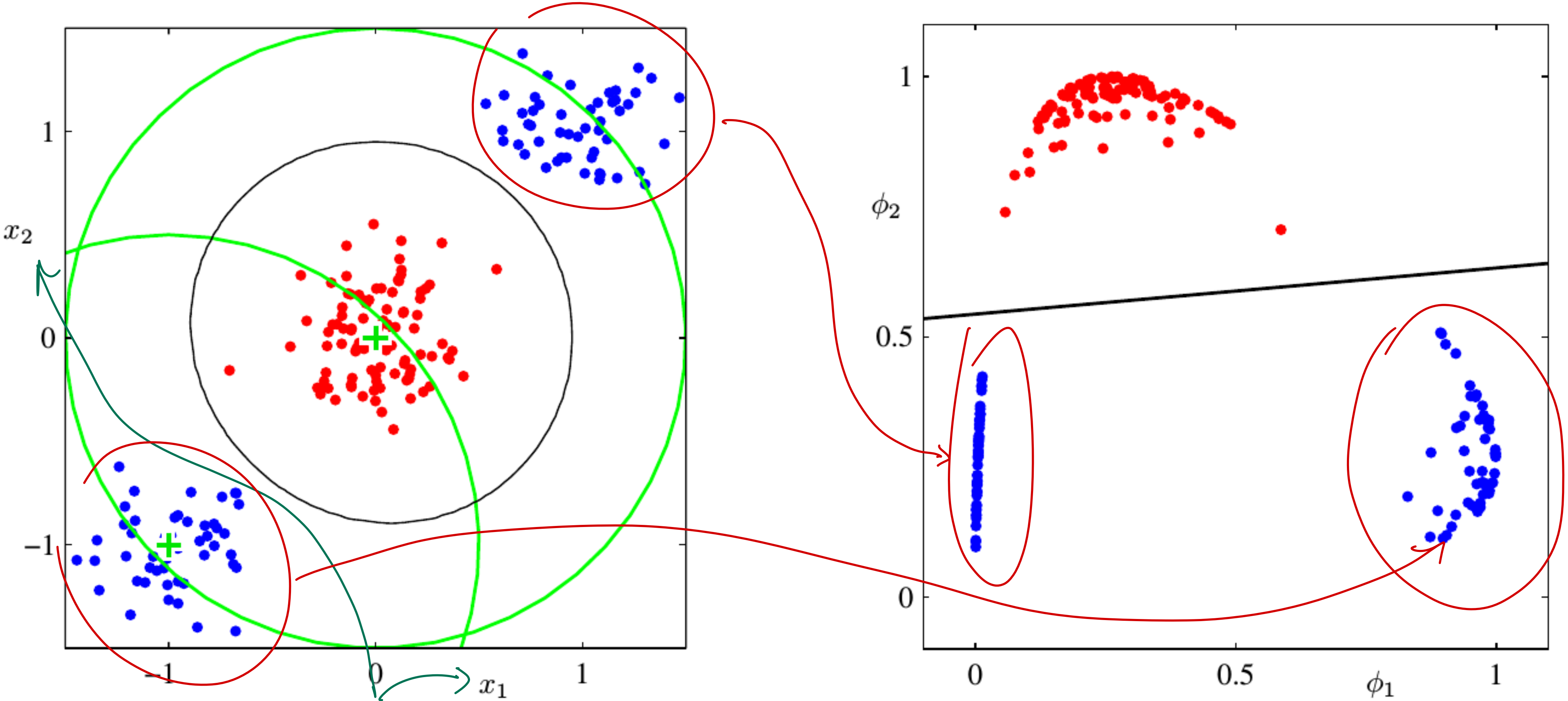
⚠

- ☒ Basically, we apply a non-linear transformation to map the **input space** into a **feature space**
- ☒ As a result, decision boundaries that are **linear** in the **feature space** would correspond to **nonlinear** boundaries in the **input space**
- ☒ This allows to apply linear classification models also to problem where samples are not **linearly separable**

Parenthe-
sis

Linear Basis Function Models: an example

- ❑ Assuming two Gaussian basis functions (in green)



INPUT SPACE NOT LINEARLY SEPARABLE

FEATURE SPACE LINEARLY SEPARABLE

2nd method

Perceptron

SO: HOW CAN WE FIND THE VECTOR w?

- The **perceptron** is a linear discriminant model proposed by Rosenblatt in 1958 along with a **sequential learning** algorithm
- Perceptron is devised for a two-class problem, where classes encoding is {-1,1}

$$f(\mathbf{x},\mathbf{w}) = \begin{cases} +1, & \text{if } \overbrace{\mathbf{w}^T \underline{\boldsymbol{\phi}(\mathbf{x})}}^{y(x)} \geq 0 \\ -1, & \text{otherwise} \end{cases}$$

we use a feature space of any type.

- The **perceptron algorithm** aims at finding a **decision surface** (also called **separating hyperplane**) by minimizing the distance of **misclassified samples** to the boundary
- Minimization of this loss function can be performed using **stochastic gradient descent**
- Despite a simpler loss function could be used in principle (e.g., number of misclassified samples), this are more complex to minimize.

2nd method

Perceptron Criterion

- ❑ We aim at finding $\mathbf{w}$ such that $\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) \geq 0$ for $\mathbf{x}_i \in C_1$ and $\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i)<0$ otherwise
- ❑ The **Perceptron Criterion** is defined as:

$$L_P(\mathbf{w}) = \underset{\text{to make } L_p \text{ positive}}{-} \sum_{n\in\mathcal{M}} \overbrace{\mathbf{w}^T\phi(\mathbf{x}_n)}^{y(x_n)} t_n \rightarrow$$

(if misclassified

→ $y(x_n)<0$ and $t_n>0$;

→ $y(x_n)>0$ and $t_n<0$.

- ▶ samples clssified correctly do not contribute to L
- ▶ each misclassified sample $\mathbf{x}_i \in \mathcal{M}$ contributes as $\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i)t_i$

set of misclassified samples.

- ❑ L_P can be minimized using **stochastic gradient descent**:

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \alpha\nabla L_P(\mathbf{w}) = \mathbf{w}^{(k)} + \underset{\text{learning rate}}{\alpha}\boldsymbol{\phi}(\mathbf{x}_n)t_n$$

- ▶ Since the scale of $\mathbf{w}$ does not change the perceptron function, usually the **learning rate** α is set to 1

2nd method

Perceptron Algorithm

Given $\mathcal{D} = \{\mathbf{x}_i, \mathbf{t}_i\}$, where i=1,...,N

```
Initialize $\mathbf{w}_0$
k ← 0
repeat
   k ← k+1
   n ← k mod N
   if $\hat{t_n} \neq t_n$ then
         $\mathbf{w}_{k+1} \leftarrow \mathbf{w}_k + \boldsymbol{\phi}(\boldsymbol{x_n}) t_n$
   endif
until convergence
```

$\hat{t}_n = f(x_n)$

The algorithm works **only** if it is possible to perfectly separate the points (with no error) via a linear boundary.

otherwise : no convergence //

2^{nd} method

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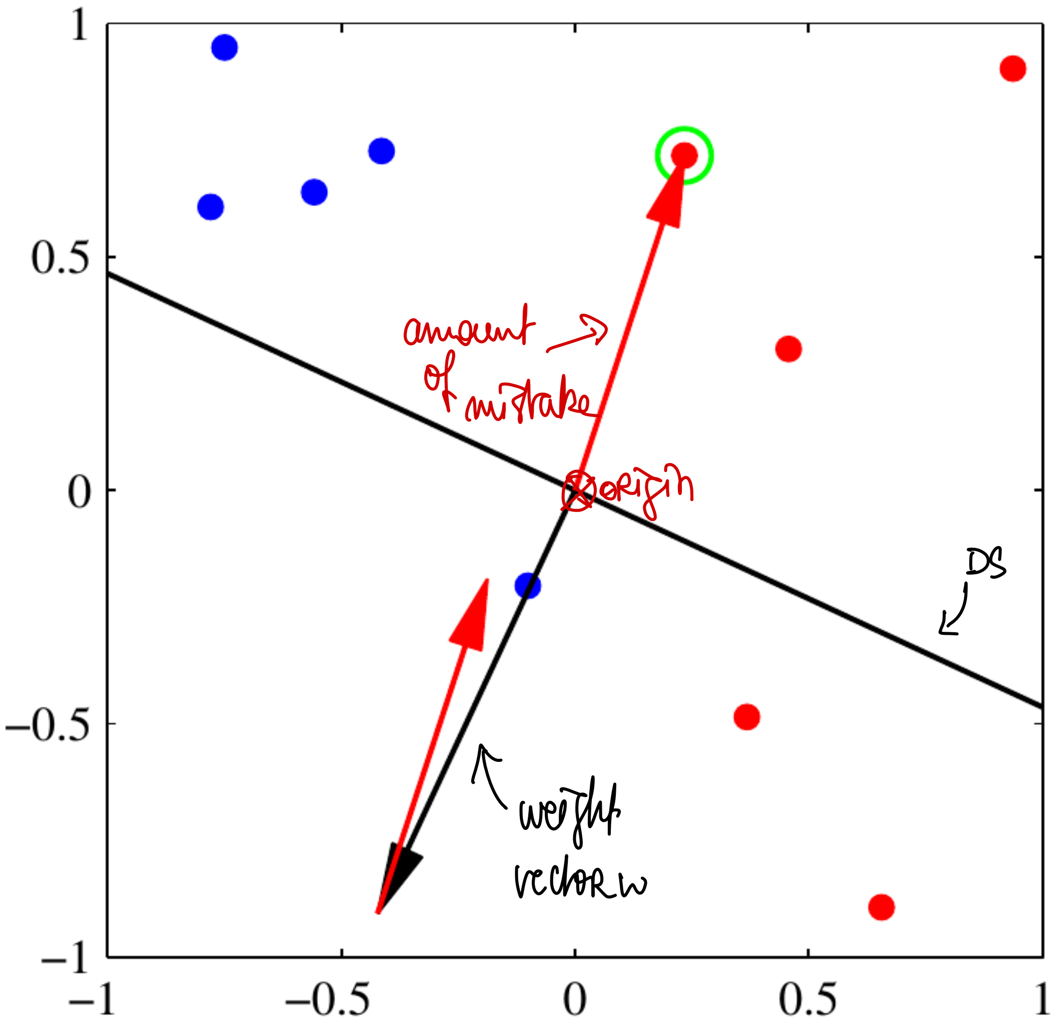

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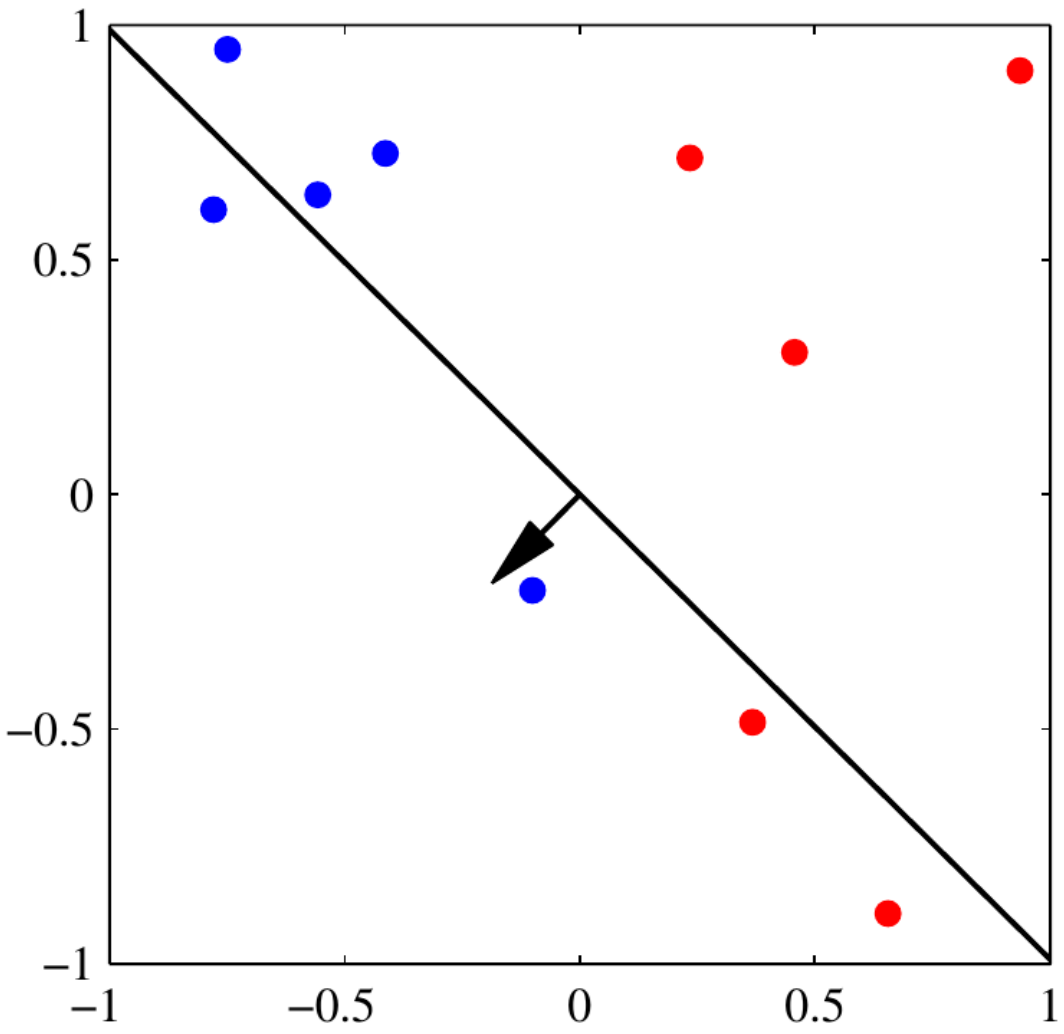

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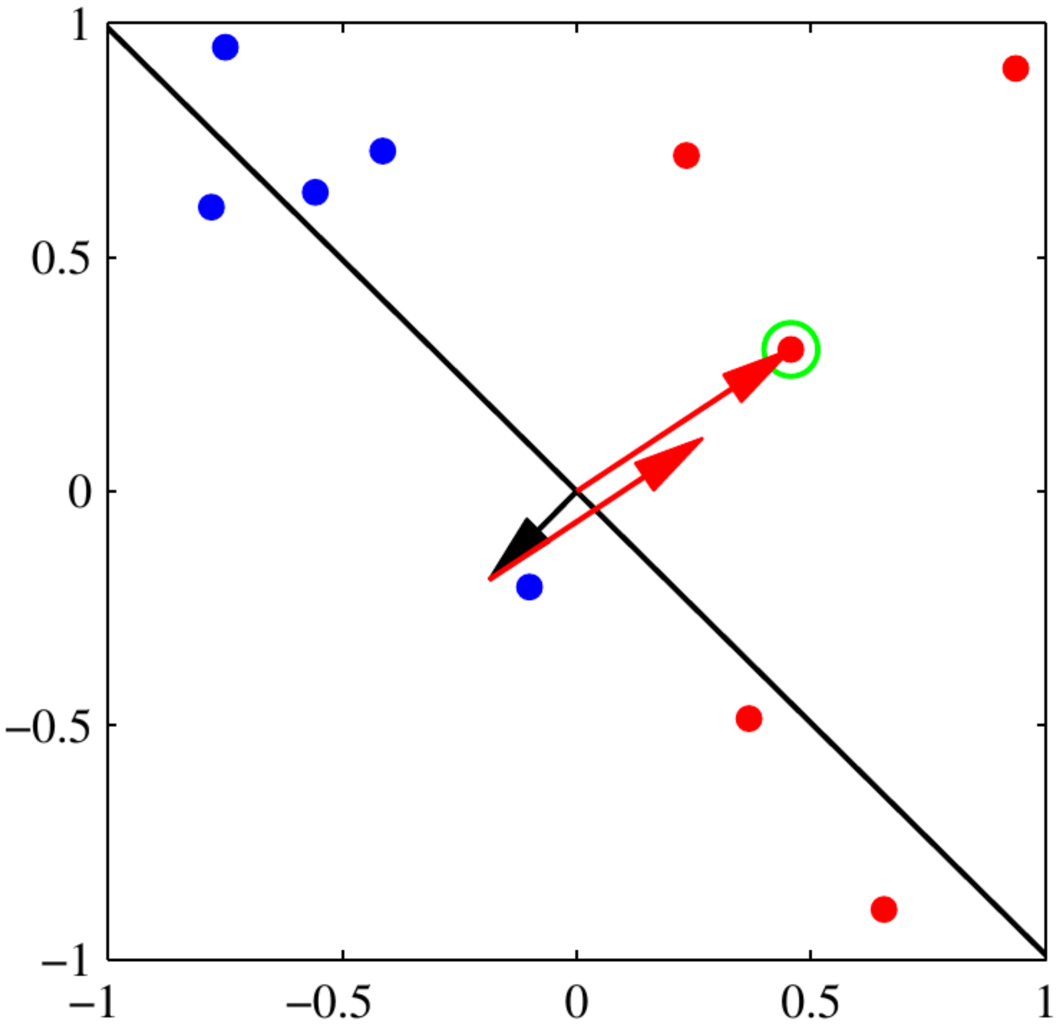

2nd method

Perceptron Algorithm

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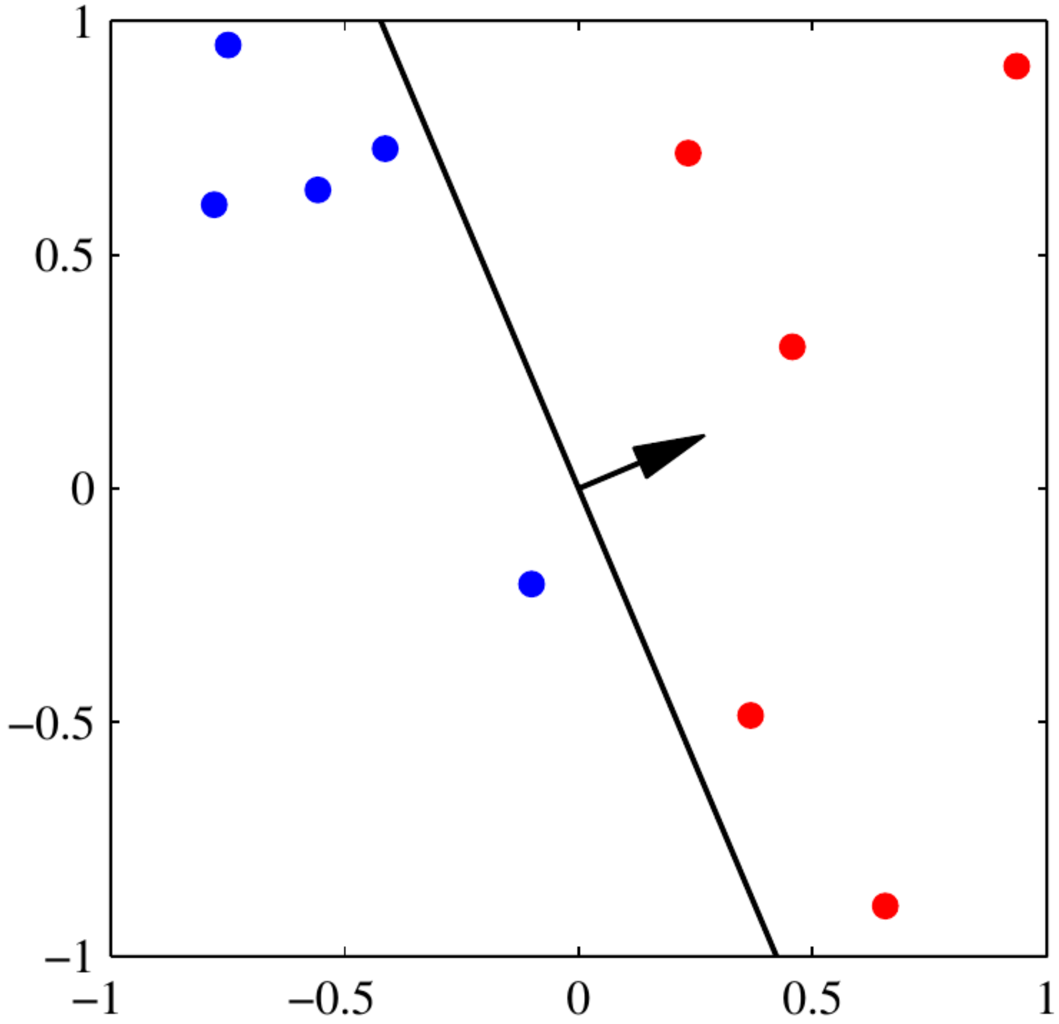


Perceptron Convergence Theorem

⚠

- A single update **reduce the error** on the **single** misclassifed sample:

$$-{\mathbf{w}^{(k+1)}}^T\phi(\mathbf{x}_n)t_n = -{\mathbf{w}^{(k)}}^T\phi(\mathbf{x}_n)t_n - (\phi(\mathbf{x}_n)t_n)^T\phi(\mathbf{x}_n)t_n < -{\mathbf{w}^{(k)}}^T\phi(\mathbf{x}_n)t_n$$

  - This does **not** imply that the entire loss is reduced after each update

We have no garanty that we are progressing @ each step...

- Perceptron Convergence Theorem:

*If the training data set is **linearly separable** in the feature space $\boldsymbol{\Phi}$, then the perceptron learning algorithm is guaranteed to find an **exact solution** in a **finite number of steps**.*

  - How many steps? Several steps might be necessary, thus it might be difficult to distinguish between **nonseparable** problems and **slowly converging** ones

⚠

  - Which solution? If **multiple solutions** exist, the one found by the algorithms depends from **initialization** of parameters and the **order** of updates

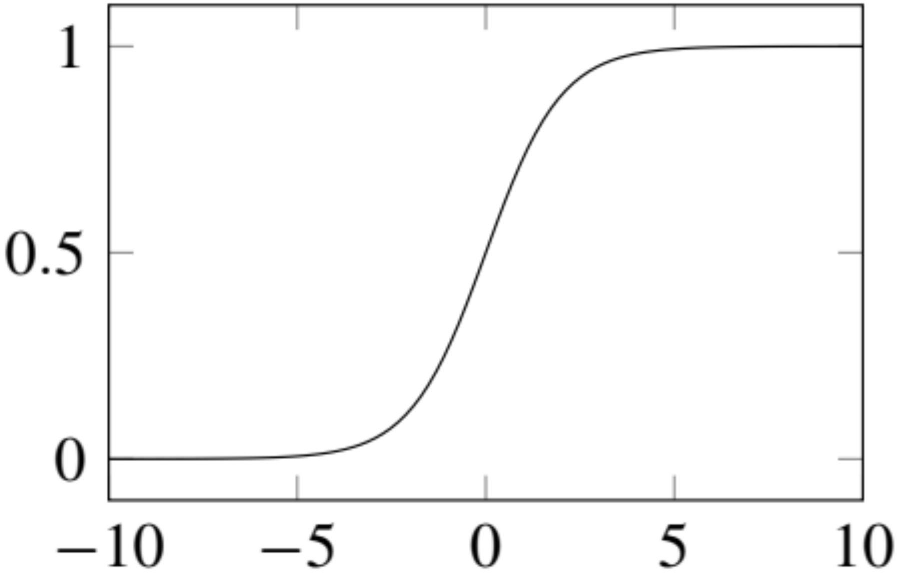
Probabilistic Discriminative Approaches

Two-Class Logistic Regression

- In a discriminative approach we model directly the conditioned class probability:

$$p(C_1|\boldsymbol{\phi}) = \frac{1}{1 + \exp(-\mathbf{w}^T\boldsymbol{\phi})} = \sigma(\mathbf{w}^T\boldsymbol{\phi})$$

  - where $\sigma(a) = 1/(1 + \exp(-a)$ is the sigmoidal function
  - $\mathrm{p}(C_2|\phi) = 1 - p(C_1|\phi)$
  - this model is knonw as logistic regression



Maximum Likelihood for Logistic Regression

- Given dataset $\mathcal{D} = \{\mathbf{x}_i, t_i\}$, where i=1,...,N and $t_i \in \{0,1\}$ we want to maximize the likelihood, i.e., the probability to observe the targets given the inputs: $p(\mathbf{t}|\mathbf{X},\mathbf{w})$

Maximum Likelihood for Logistic Regression

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- ❑ We model the likelihood of the single sample using a Bernoulli distribution, using the logistic regression model for conditioned class probability:

$$p(t_n|\mathbf{x}_n, \mathbf{w}) = \underbrace{y_n^{t_n}(1-y_n)^{1-t_n}}_{= p(t_n=1|x_n,w) \text{ if } t_n = 1 \text{ \& otherwise } 1-p(t_n=1|X_n,w).} \quad \text{where} \quad y_n = p(t_n = 1|\mathbf{x}_n, \mathbf{w}) = \sigma(\mathbf{w}^T \boldsymbol{\phi}_n)$$

- ❑ Assuming that data in $\mathcal{D}$ have been independently sampled we get:

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n}(1-y_n)^{1-t_n}, \quad y_n = \sigma(\mathbf{w}^T \boldsymbol{\phi}_n)$$

Maximum Likelihood for Logistic Regression (2)

- A convenient loss function to **minimize** is the negative log-likelihood (also **known as “cross-entropy error” function**)

$$L(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = -\sum_{n=1}^{N} (t_n \ln y_n + (1 - t_n) \ln(1 - y_n)) = \sum_{n=1}^{N} L_n$$

- Now we have to compute the derivative of $L(\mathbf{w})$:

$$\frac{\partial L_n}{\partial y_n} = \frac{y_n - t_n}{y_n(1 - y_n)}, \qquad \frac{\partial y_n}{\partial \mathbf{w}} = y_n(1 - y_n)\boldsymbol{\phi}_n,$$

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$$\frac{\partial L_n}{\partial y_n} = \frac{y_n - t_n}{y_n(1 - y_n)}, \quad \frac{\partial y_n}{\partial \mathbf{w}} = y_n(1 - y_n)\boldsymbol{\phi}_n, \underset{\overset{\uparrow}{\text{Chain rule}}}{\Longrightarrow} \frac{\partial L_n}{\partial \mathbf{w}} = \frac{\partial L_n}{\partial y_n}\frac{\partial y_n}{\partial \mathbf{w}} = (y_n - t_n)\boldsymbol{\phi}_n$$

Maximum Likelihood for Logistic Regression (3)

- Thus the gradient of the loss function is:

$$\nabla L(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n)\phi_n$$

- due to the nonlinear logistic regression function it is not possible to find a closed-form solution
- however, the error function is **convex** and **gradient-based optimization** can be applied (also in an **online learning setting**)

Multiclass Logistic Regression

$k>2$

□ In multiclass problems, $p(C_k|\boldsymbol{\phi})$ is modeled by a **softmax** tranformation of the output of K linear functions (one for each class):

$$p(C_k|\boldsymbol{\phi}) = y_k(\boldsymbol{\phi}) = \frac{\exp(\mathbf{w}_k{}^T\boldsymbol{\phi})}{\sum_j \exp(\mathbf{w}_j{}^T\boldsymbol{\phi})}$$

□ As for the two-class logistic regression and assuming 1-of-K encoding for the target, we can compute **likelihood** as:

$$p(\mathbf{T}|\boldsymbol{\Phi}, \mathbf{w}_1, \dots, \mathbf{w}_K) = \prod_{n=1}^{N} \underbrace{\left(\prod_{k=1}^{K} p(C_k|\boldsymbol{\phi}_n)^{t_{nk}}\right)}_{\text{Only one term corresponding to correct class}} = \prod_{n=1}^{N}\left(\prod_{k=1}^{K} y_{nk}^{t_{nk}}\right)$$

$T = (t_1, t_2, \dots, t_N)$

Multiclass Logistic Regression

- In multiclass problems, $p(C_k|\boldsymbol{\phi})$ is modeled by a **softmax** tranformation of the output of K linear functions (one for each class):

$$p(C_k|\boldsymbol{\phi}) = y_k(\boldsymbol{\phi}) = \frac{\exp(\mathbf{w}_k{}^T\boldsymbol{\phi})}{\sum_j \exp(\mathbf{w}_j{}^T\boldsymbol{\phi})}$$

- As for the two-class logistic oding for the target, we can compute **likelihood** as:

$$y_{nk} = p(C_k|\boldsymbol{\phi}_n) = \frac{\exp(\mathbf{w}_k{}^T\boldsymbol{\phi}_n)}{\sum_j \exp(\mathbf{w}_j{}^T\boldsymbol{\phi}_n)}$$

$$p(\mathbf{T}|\boldsymbol{\Phi}, \mathbf{w}_1, \ldots, \mathbf{w}_K) = \prod_{n=1}^{N} \underbrace{\left(\prod_{k=1}^{K} p(C_k|\boldsymbol{\phi}_n)^{t_{nk}}\right)}_{\text{Only one term corresponding to correct class}} = \prod_{n=1}^{N}\left(\prod_{k=1}^{K} y_{nk}^{t_{nk}}\right)$$

Multiclass Logistic Regression (2)

- As for the two-class problem, we can minimize the cross-entropy error function:

$$L(\mathbf{w}_1, \ldots, \mathbf{w}_K) = -\ln p(\mathbf{T}|\mathbf{\Phi}, \mathbf{w}_1, \ldots, \mathbf{w}_K) = -\sum_{n=1}^{N}\left(\sum_{k=1}^{K} t_{nk} \ln y_{nk}\right)$$

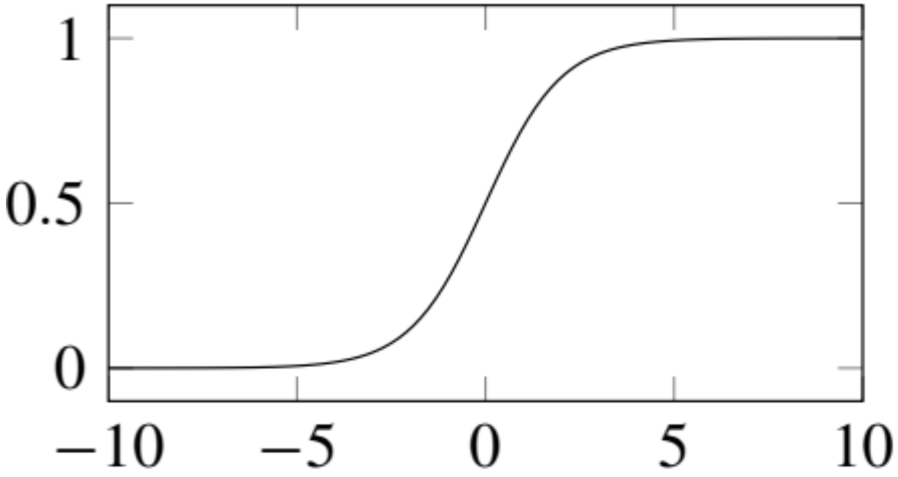
- Then, we compute the gradient for each weights vector:

$$\nabla L_{\mathbf{w}_j}(\mathbf{w}_1, \ldots, \mathbf{w}_K) = \sum_{n=1}^{N}(y_{nj} - t_{nj})\boldsymbol{\phi}_n$$

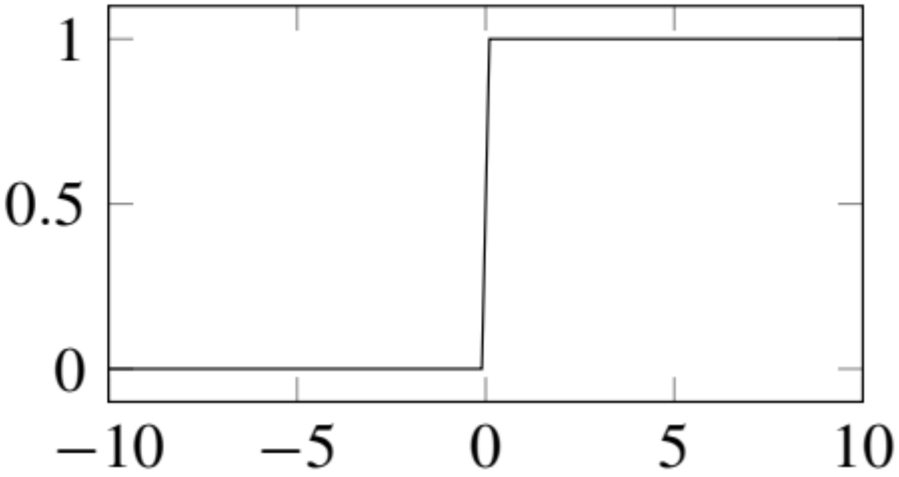
Logistic Regression and Perceptron Algorithm

ANALOG TO PERCEPTRON ALGO :

- If we replace the logistic function with a step function...



$$y(\mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \boldsymbol{\phi}(\mathbf{x})}}$$



$$y(\mathbf{x}, \mathbf{w}) = \begin{cases} 1 & \text{if } \mathbf{w} \cdot \boldsymbol{\phi}(\mathbf{x}) > 0 \\ 0 & \text{otherwise} \end{cases}$$

- ... logistic regression leads to the same **updating rule** of the perceptron algorithm:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \left(y(\mathbf{x}_n, \mathbf{w}) - t_n \right) \boldsymbol{\phi}_n$$