Linear Classifiers

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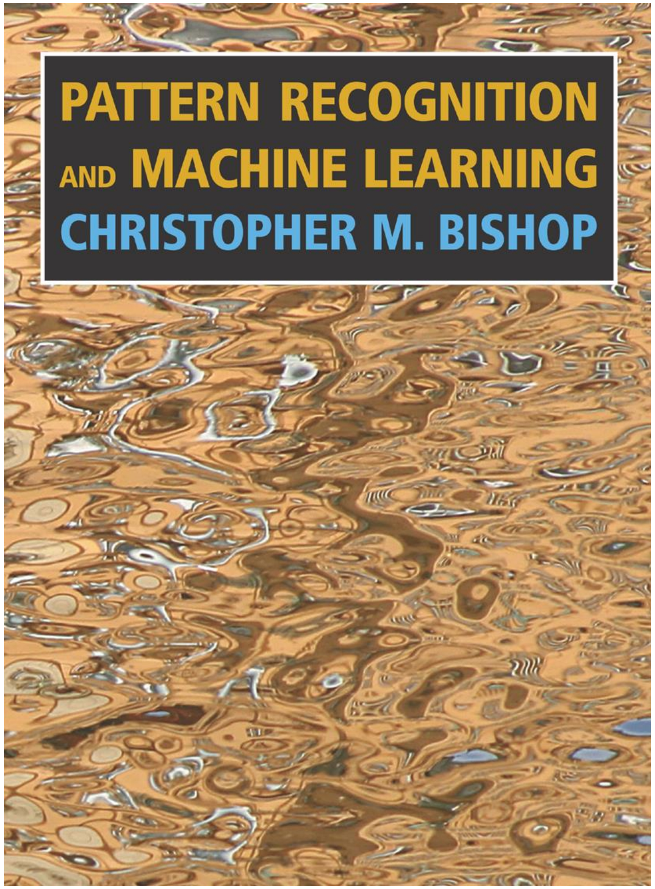
Office hour: Thursday 2-3pm

Reference



Today's class *roughly* follows Chapter 4-4.2.

Pattern Recognition and Machine Learning

Christopher Bishop, 2006

Outline

- Geometry of decision function
- **Non probabilistic classifiers**
  - Least square classifier
  - Fisher discriminant analysis
- **Probabilistic classifiers**
  - Generative Classifiers

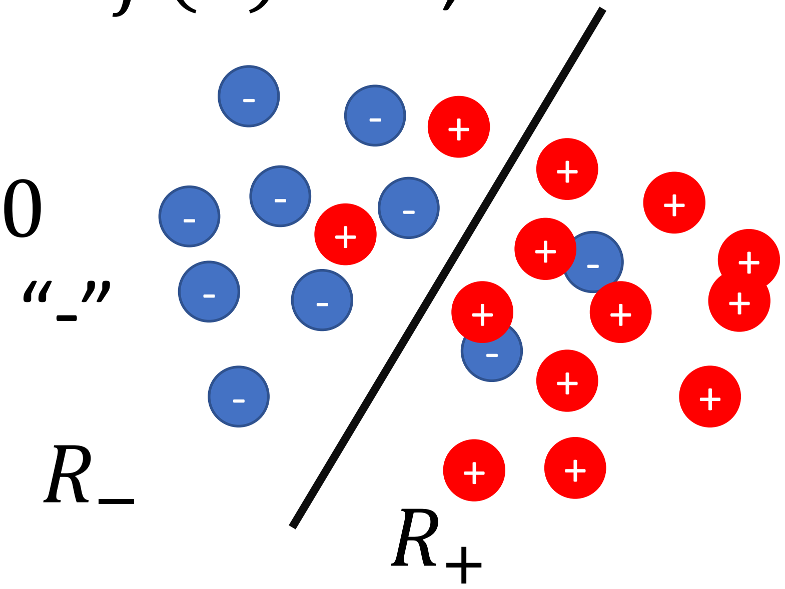
Binary Classification

- **Input**: $\{\boldsymbol{x}_i\}_{i=1}^{n}$
- **Output**: $y \in \{-1, +1\}$
- A decision boundary is defined by a function $f(\boldsymbol{x})$

$f(\boldsymbol{x}) = 0$, decision boundary

$f(\boldsymbol{x}) \leq 0$

Prediction "-"

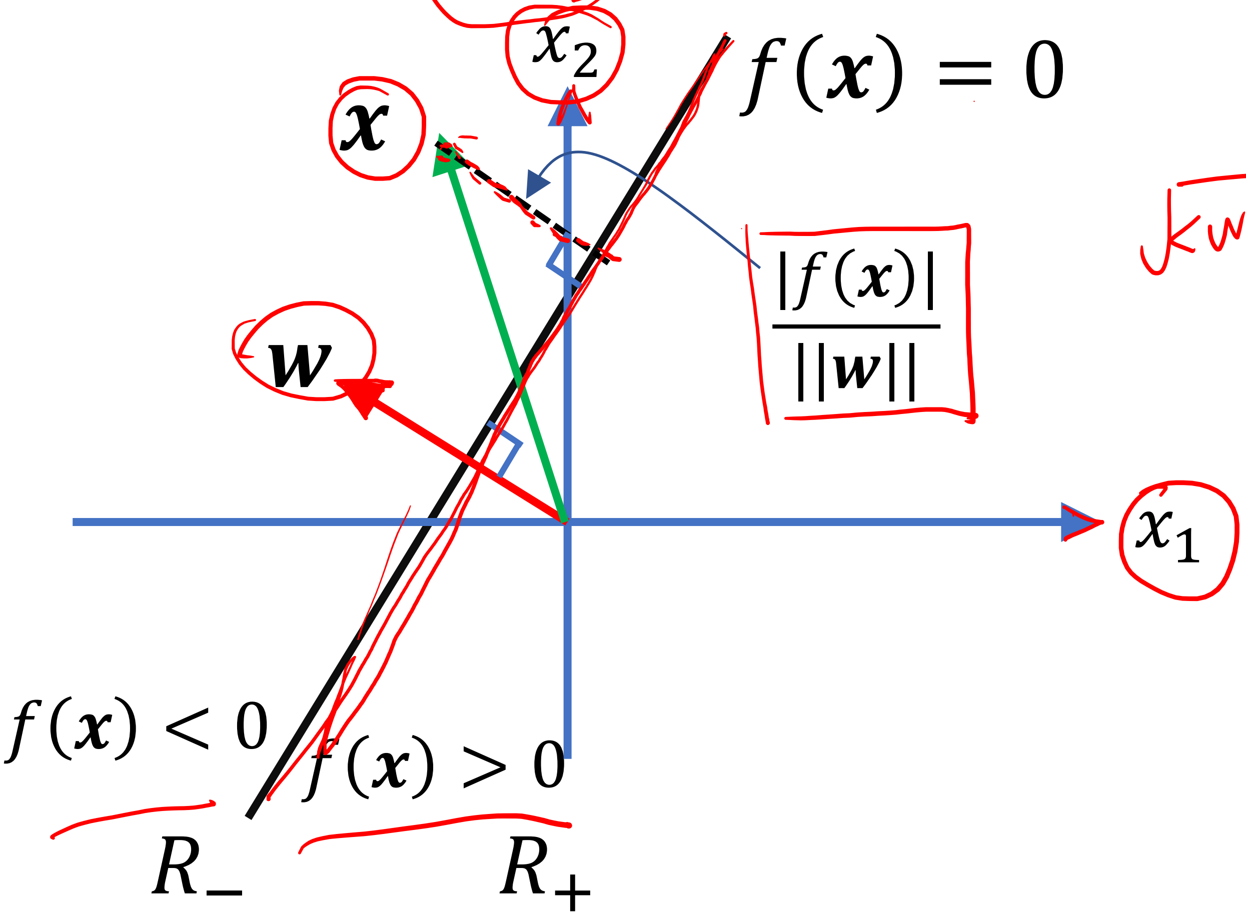


$f(\boldsymbol{x}) \geq 0$

Prediction "+"

Geometry of Binary Classification

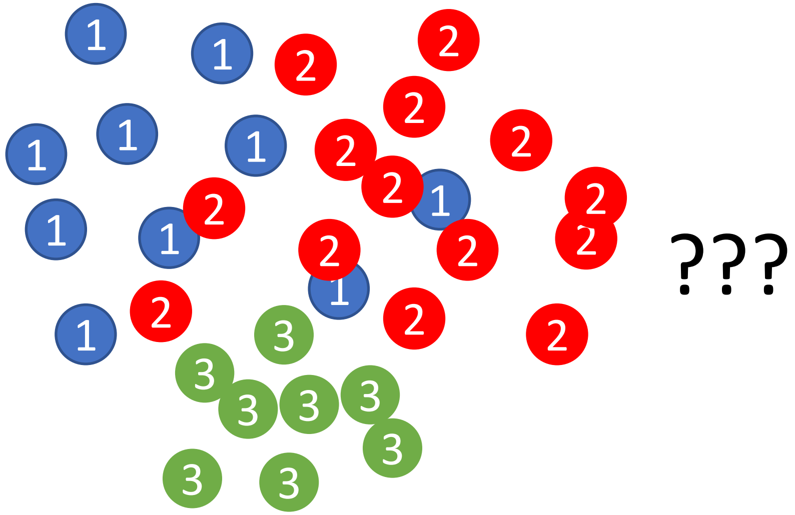
Suppose $f(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + w_0$



$\sqrt{\langle w, w \rangle}$

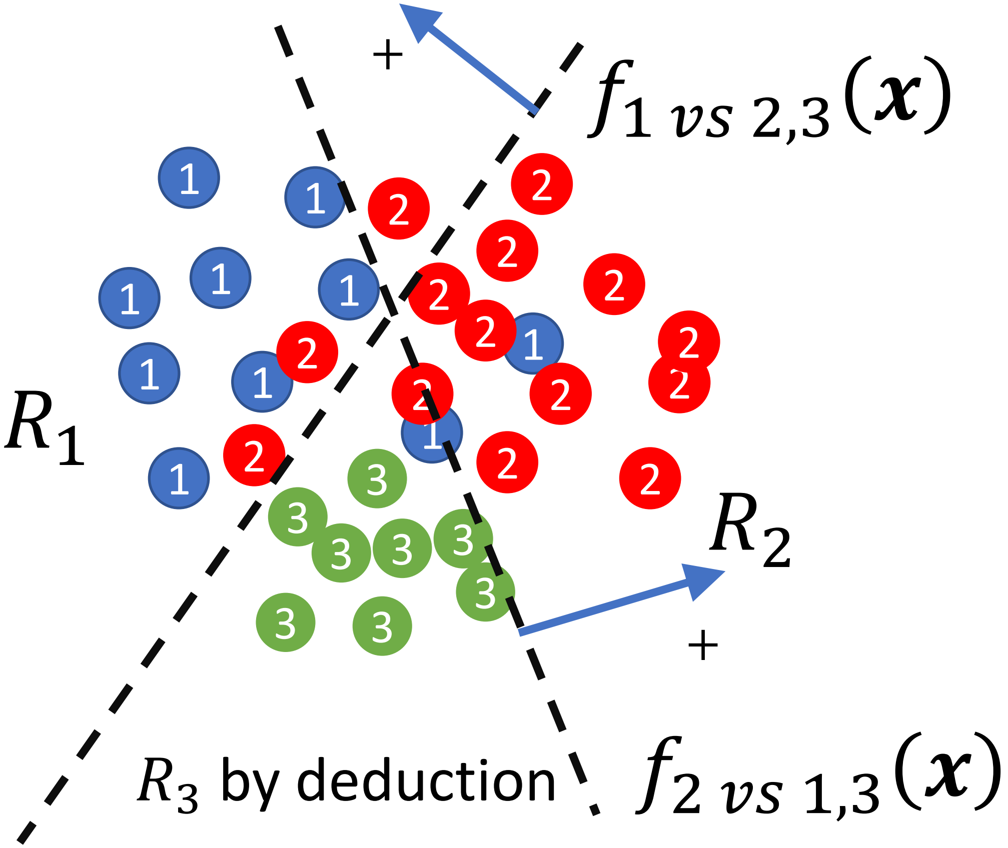
Multi-class Classification

- **Input:** $\{\boldsymbol{x}_i\}_{i=1}^{n}$
- **Output:** $y \in \{1 \ldots K\}$
- The geometry gets a lot more complicated…
  - Cannot simply check the sign of a single $f(\boldsymbol{x})$.



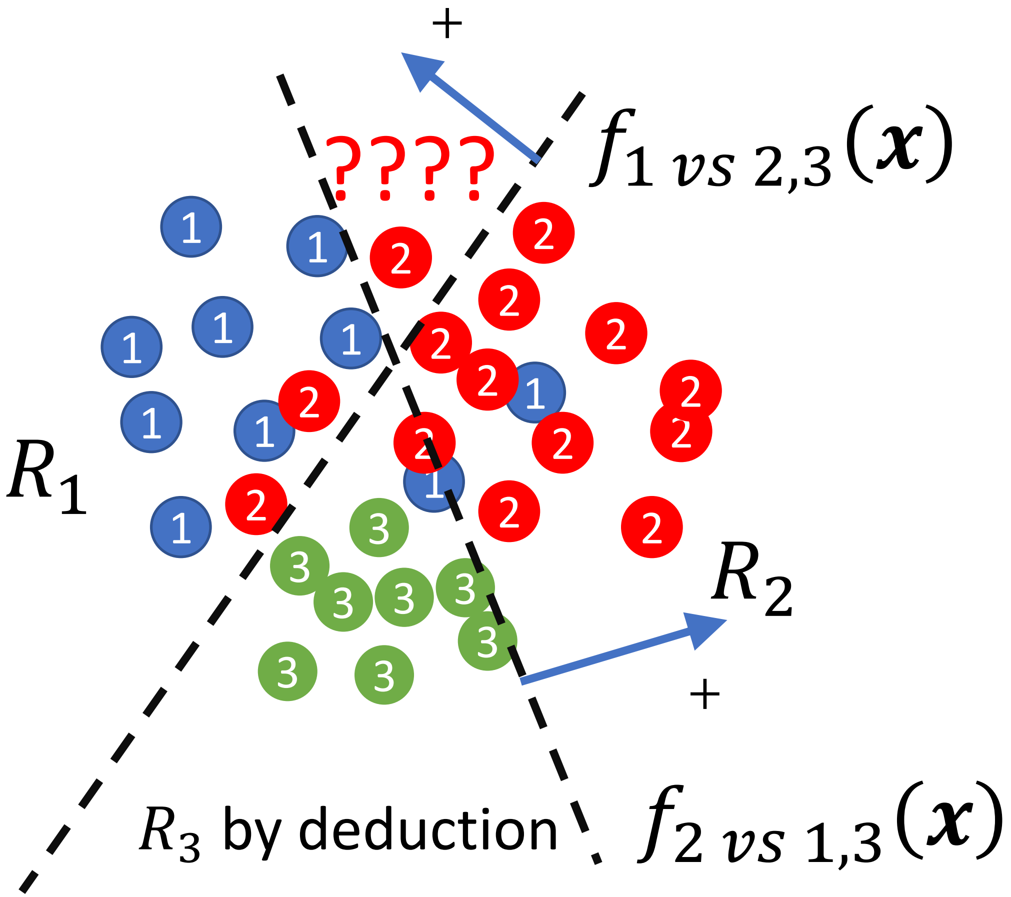
One versus The Other

- Construct $K-1$ classifier
- Classify Class k vs. the rest of classes


+
$f_{1\ vs\ 2,3}(\boldsymbol{x})$
1
2
3
R_1
R_2
+
R_3 by deduction
$f_{2\ vs\ 1,3}(\boldsymbol{x})$

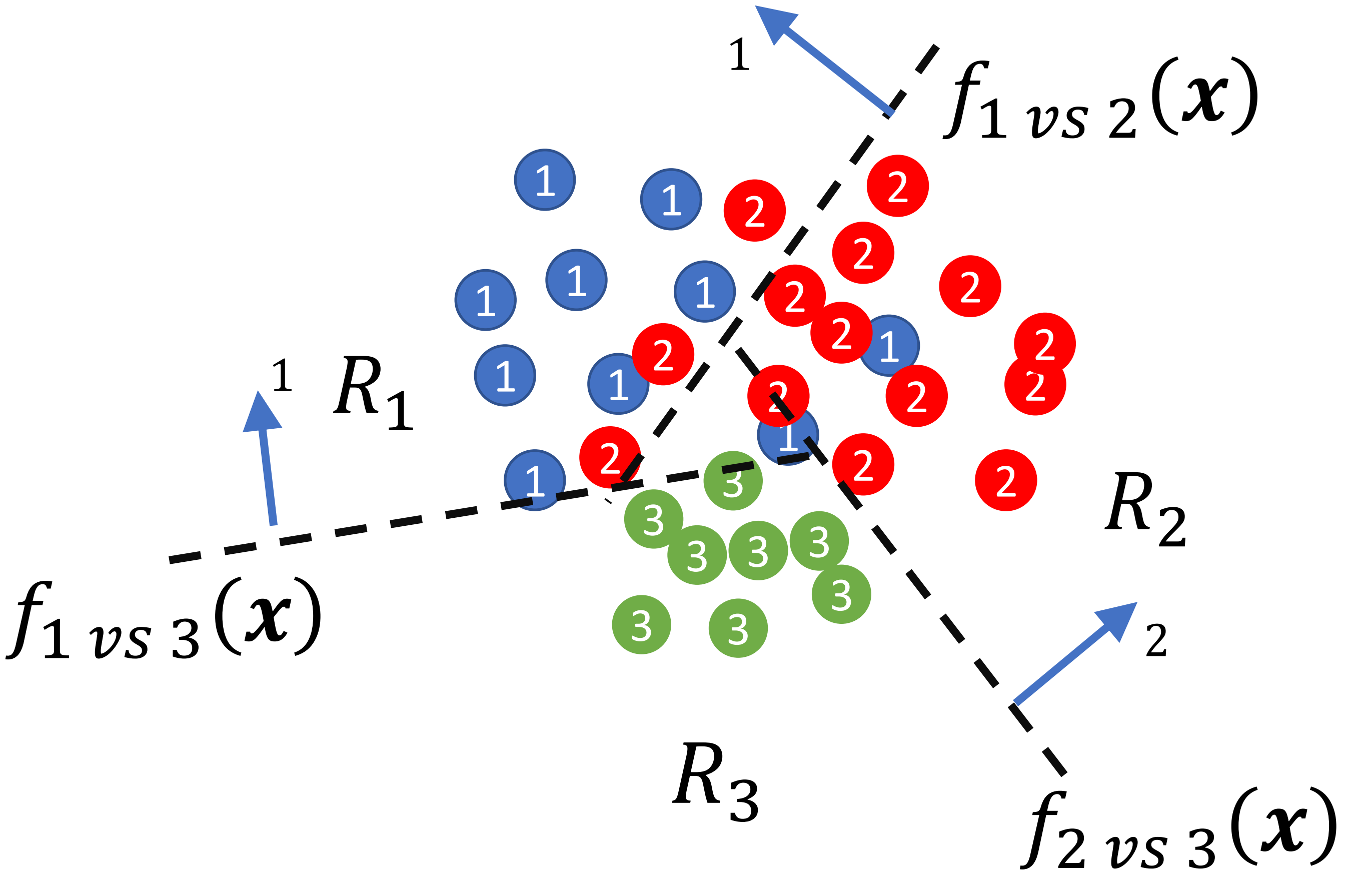
One versus The Other

- One versus the other also creates confusion!


+
????
$f_{1\ vs\ 2,3}(\boldsymbol{x})$
R_1
R_2
+
R_3 by deduction
$f_{2\ vs\ 1,3}(\boldsymbol{x})$

One versus One

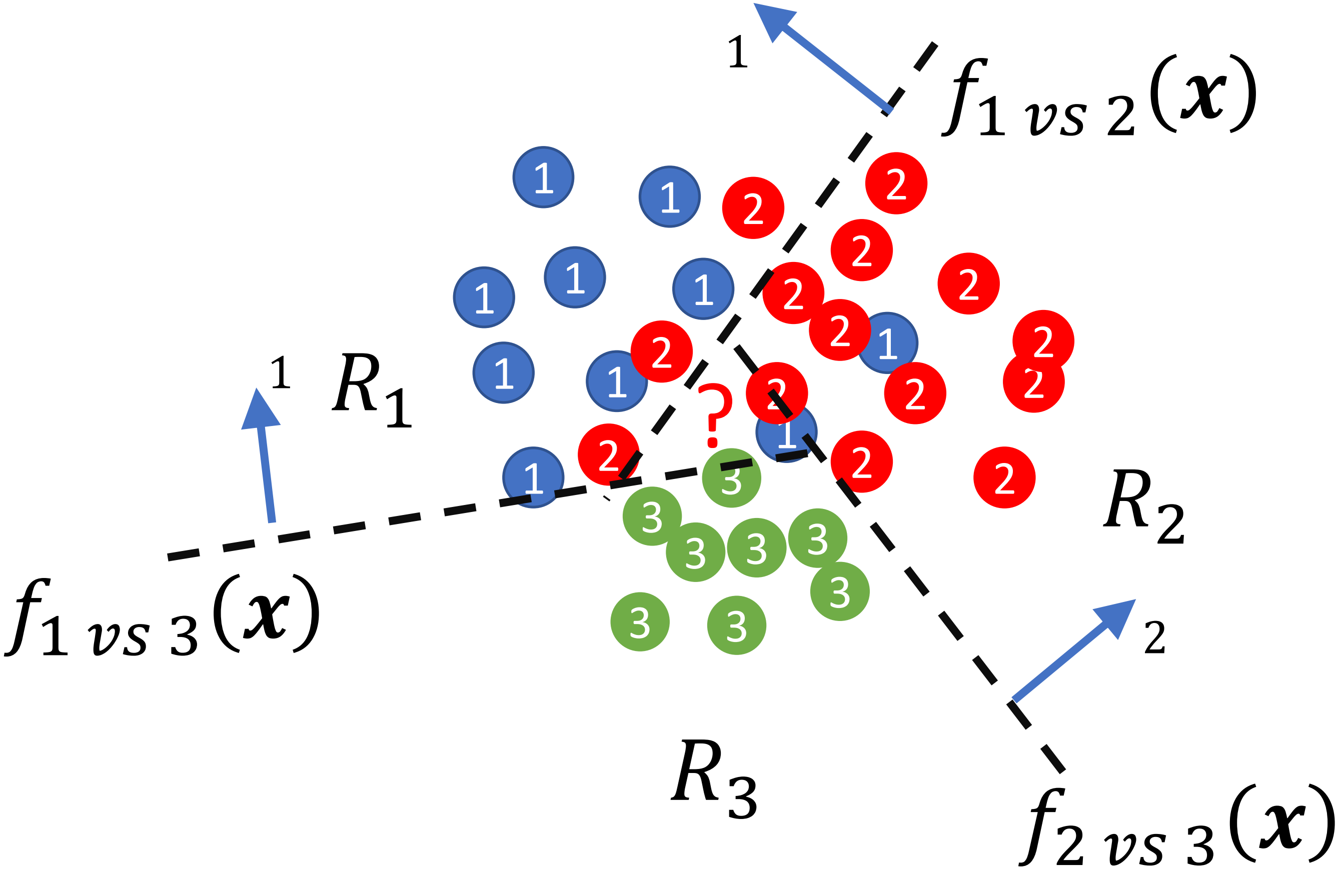
- We can create pairwise classifiers and check majority vote.



1
$f_{1\ vs\ 2}(\boldsymbol{x})$
1
R_1
R_2
2
$f_{1\ vs\ 3}(\boldsymbol{x})$
R_3
$f_{2\ vs\ 3}(\boldsymbol{x})$

One versus One

- One versus one creates confusion as well…


1
$f_{1\ vs\ 2}(\boldsymbol{x})$
1
R_1
?
R_2
$f_{1\ vs\ 3}(\boldsymbol{x})$
2
R_3
$f_{2\ vs\ 3}(\boldsymbol{x})$

Multi-class Classification

- Rather than relying on sign of f to make predictions, we estimate K functions:
- $\{f_k(\boldsymbol{x};\boldsymbol{w}_k)\}_{k=1}^{K}$

- Given an $\boldsymbol{x}$, prediction is $\hat{k} = \max_k f_k\left(\boldsymbol{x};\boldsymbol{w}_j\right)$,

- **Problem**: f_k does not have a simple geometry interpretation anymore.
- However, f_k does have probabilistic interpretation.

How do we obtain the prediction function f?

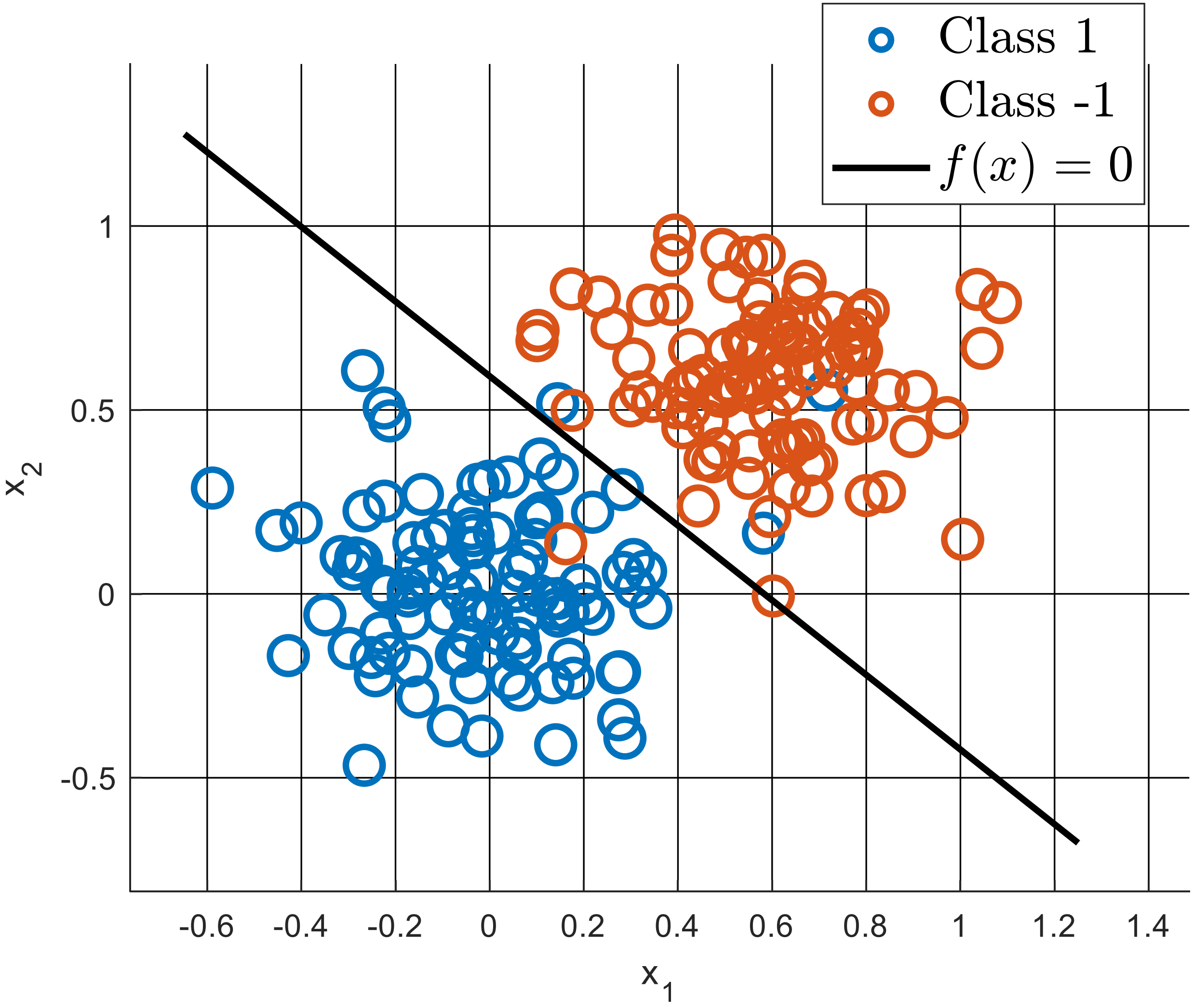
Can we use least squares?

Least Square Classifier

- For binary classification, import D in LS.
- $\boldsymbol{w}_{\mathrm{LS}} \coloneqq \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i \in D} [y_i - f(\boldsymbol{x}_i; \boldsymbol{w})]^2$
  - Now y_i takes binary value 1 or -1

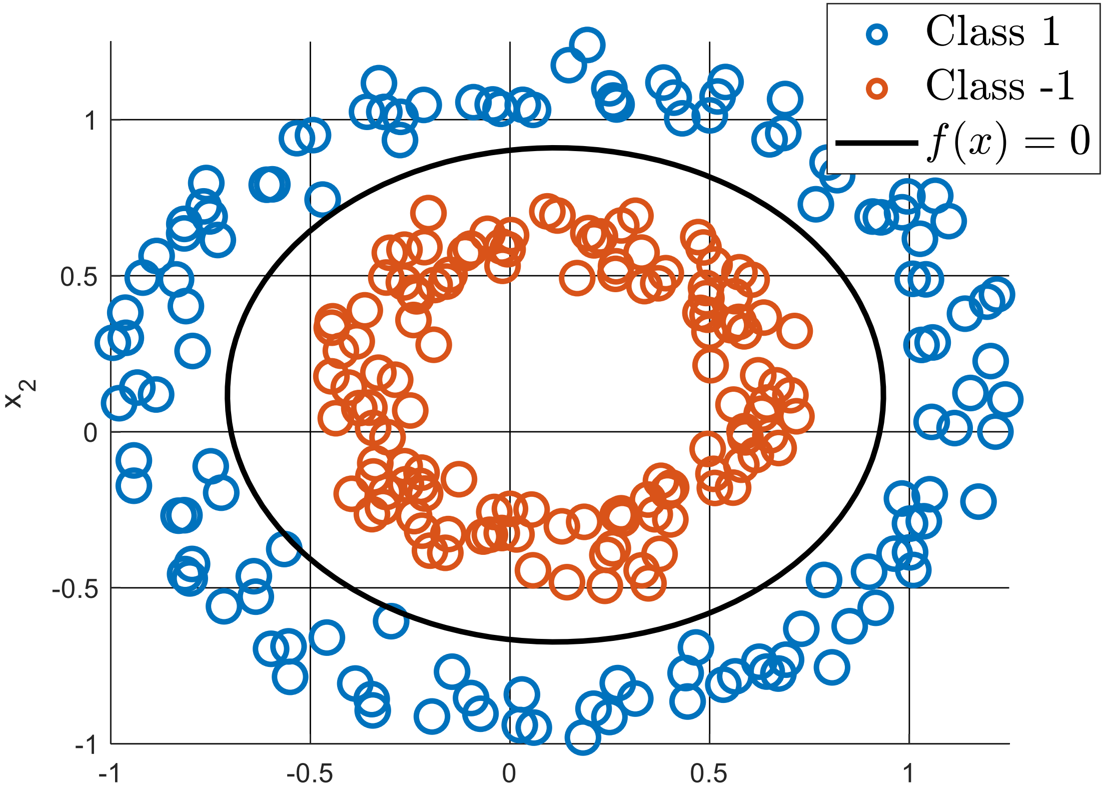
- Prediction function $f(\boldsymbol{x}_i; \boldsymbol{w}_{\mathrm{LS}})$.
- The predicted label $\hat{y} \coloneqq \operatorname{sign}\left(f(\boldsymbol{x}_i; \boldsymbol{w}_{\mathrm{LS}})\right)$

Least Square Classifier



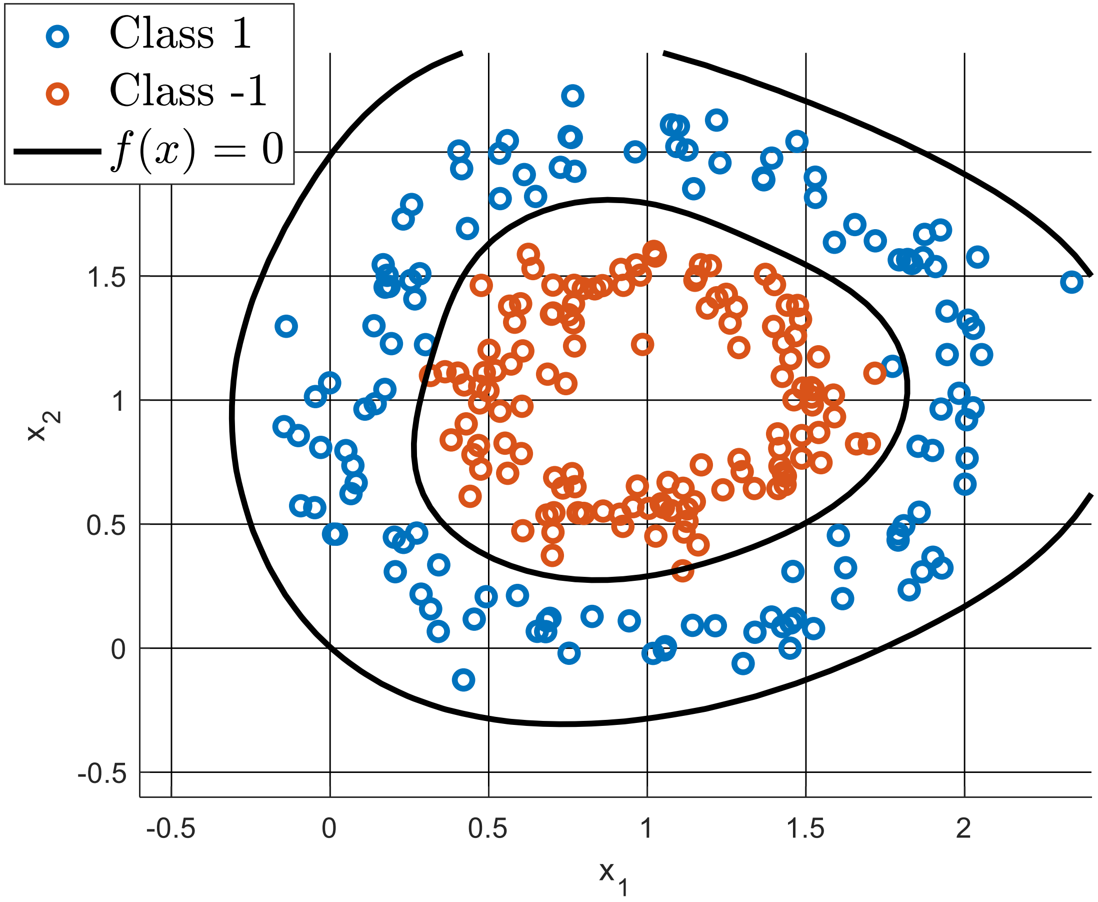
Least Square Classifier

- You can use feature transform $\boldsymbol{\phi}$ for f as well.
- $f(\boldsymbol{x};\boldsymbol{w}) \coloneqq \langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}) \rangle$,
- e.g. poly., trigonometric, RBF, kernel.



Least Square Classifier

Data may not be separable in the original space but can be separable in the **feature space** created by $\boldsymbol{\phi}$!



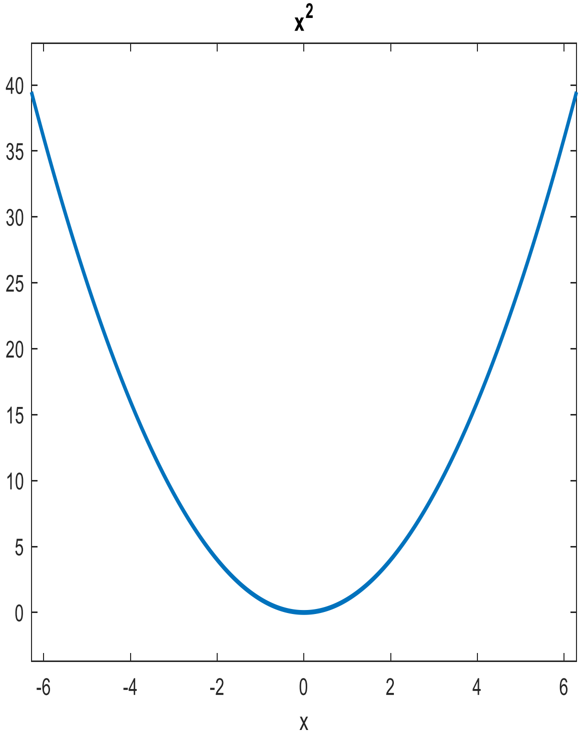
Multi-class LS classification

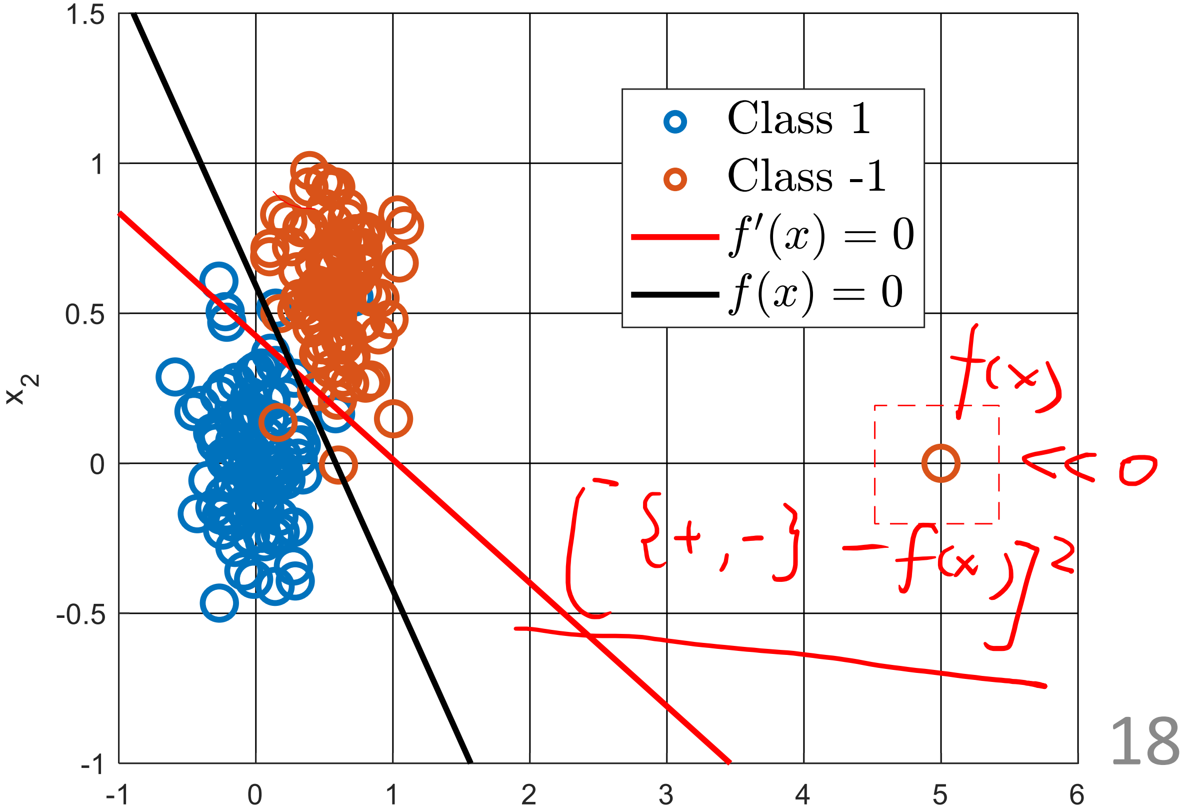
- LS can be adapted to multi-class classification.
- Suppose output $y \in \{1 \dots K\}$
- Replace $y_i = k$ in D with $\boldsymbol{t}_i \in \{0,1\}^K$.
    - $t_i^{(k)} = 1$.
    - $t_i^{(j)} = 0, \forall j \neq k$
- "**One-hot encoding**"

- $\boldsymbol{W}_{\mathrm{LS}} \coloneqq \operatorname{argmin}_{\boldsymbol{W}} \sum_{i \in D} ||\boldsymbol{t}_i - \boldsymbol{W}^\top \widetilde{\boldsymbol{X}}_i||^2$
- $\boldsymbol{W}_{\mathrm{LS}} \in R^{(d+1)\times K}, \widetilde{\boldsymbol{X}} \coloneqq \left[\boldsymbol{X}_i^\top, \mathbf{1}\right]^\top, \boldsymbol{X}_i \coloneqq [\boldsymbol{x}_i, \boldsymbol{x}_i \dots] \in R^{d\times K}$.

Why not to use LS Classifier?

- Square loss does not make sense in classification tasks.
- Data point far away from decision boundary can influence the decision boundary by a lot.





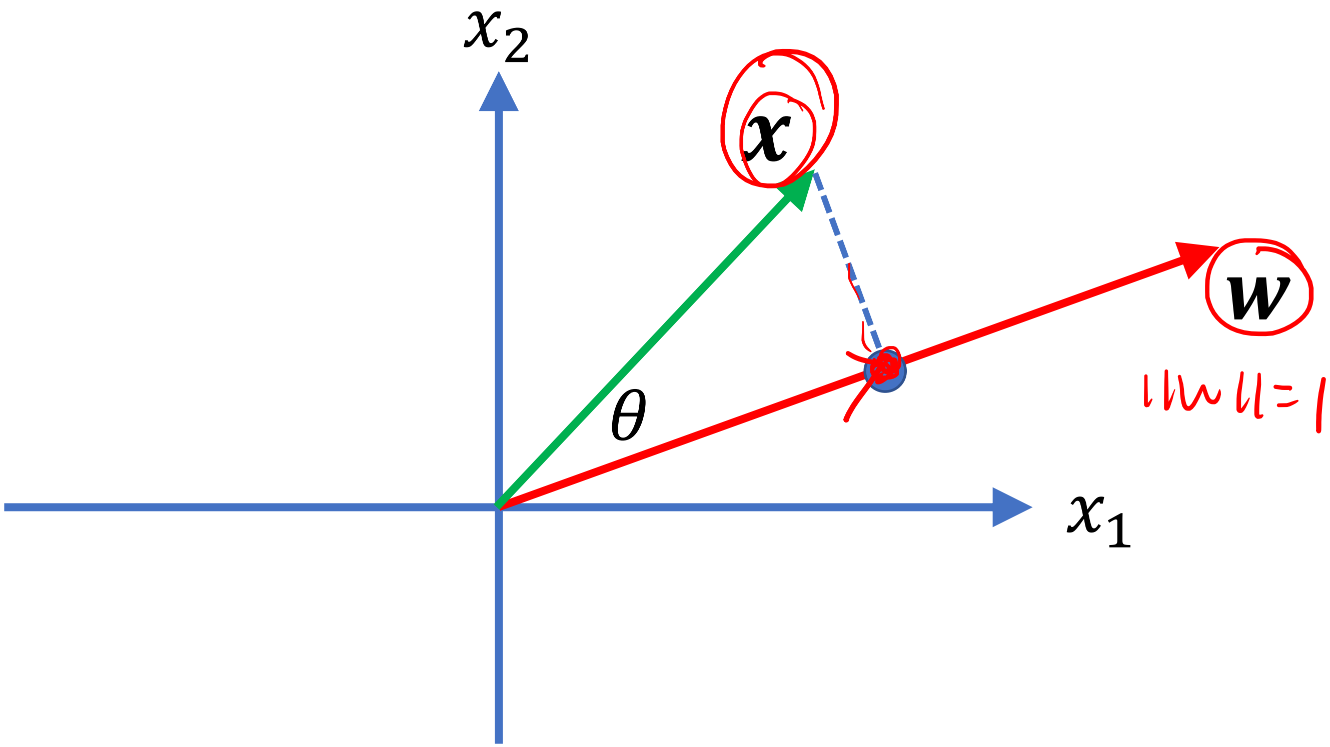
Why not to use LS Classifier?

- Unlike LS regression,
- LS classification lacks a probabilistic interpretation.
- It cannot be interpreted as Maximum Likelihood of some probabilistic model on D.

Fisher Discriminant Analysis (FDA)

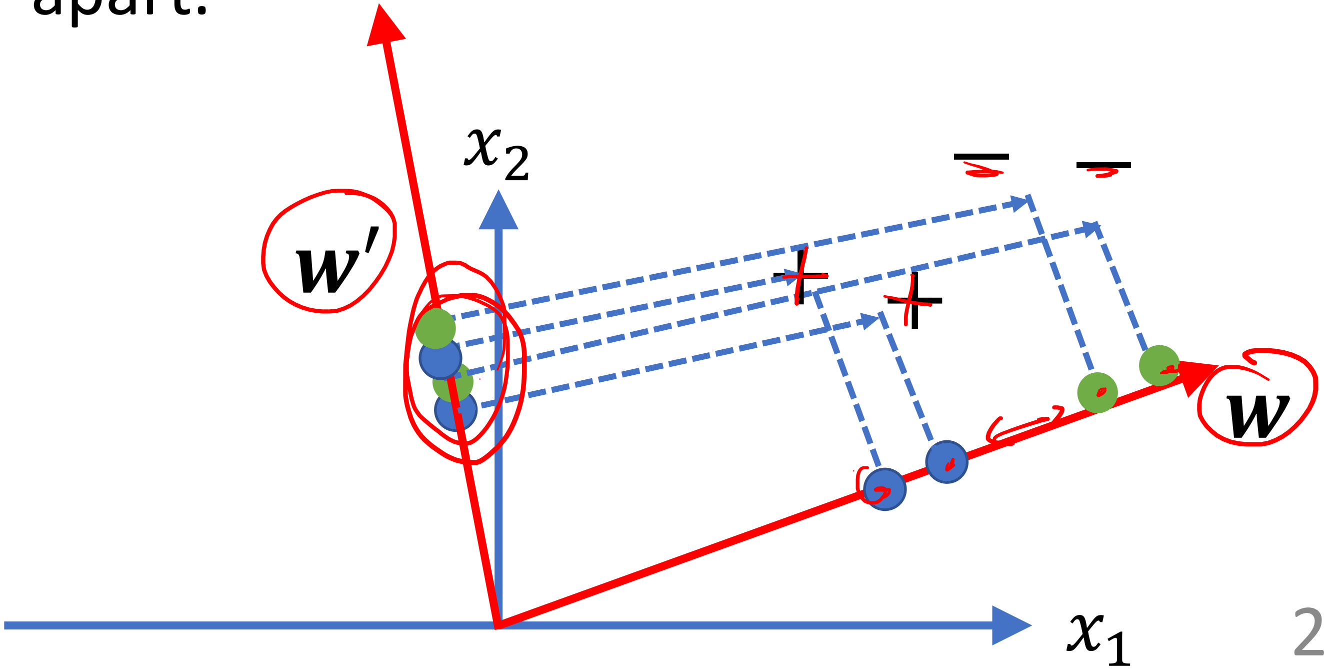
Embedding by Inner Product

- The inner product $\langle \boldsymbol{w}, \boldsymbol{x} \rangle$ "embeds" $\boldsymbol{x}$, onto a one-dimensional line along $\boldsymbol{w}$ direction.



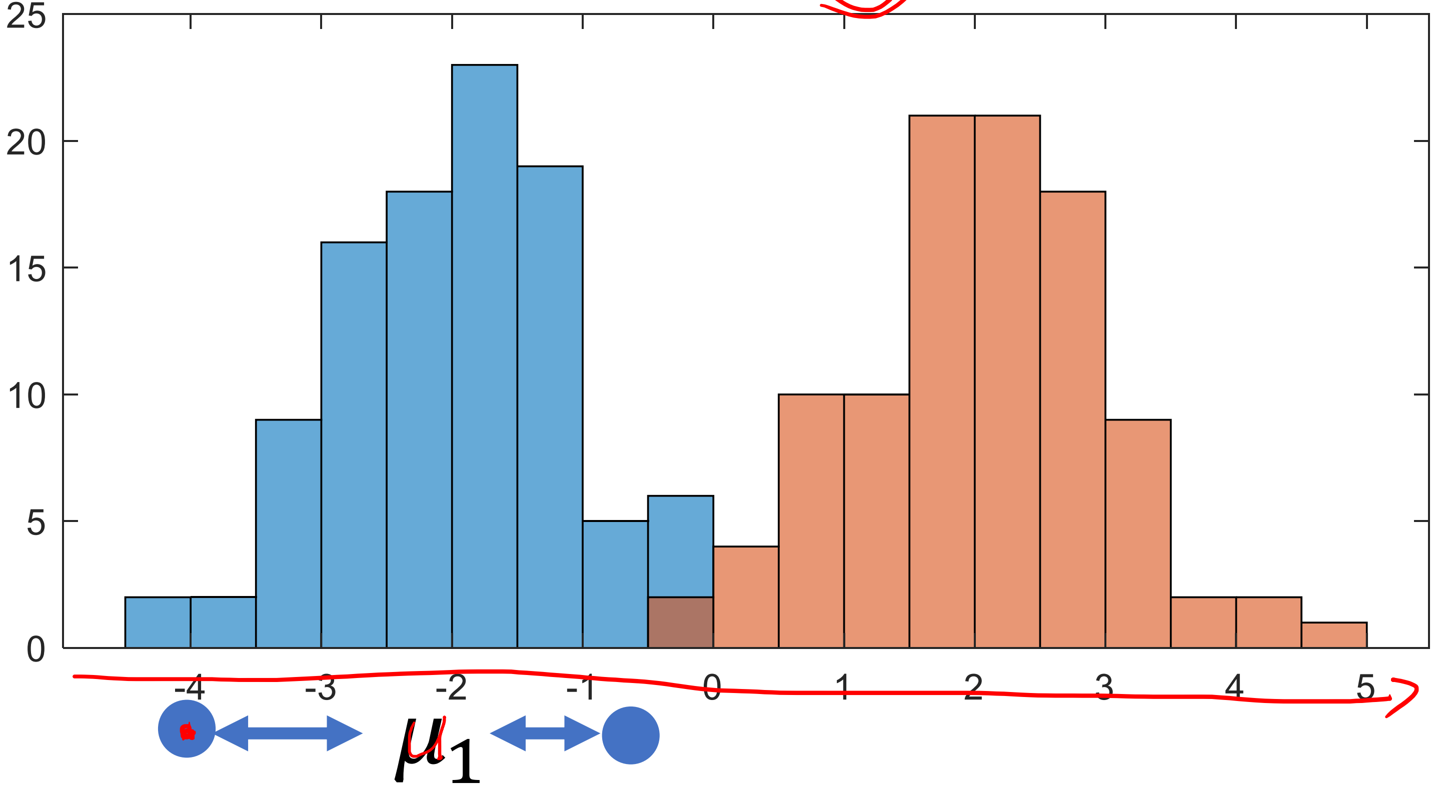
Embedding by Inner Product

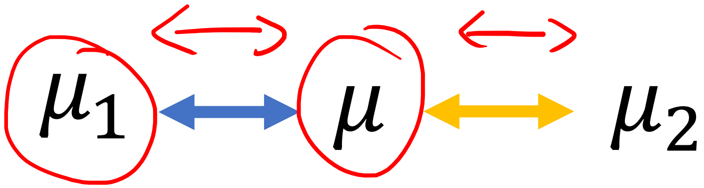
- What would be a good embedding?
- Clearly, we prefer $\boldsymbol{w}$ to $\boldsymbol{w}'$, as the embedding is **more separated** between $+$ and $-$.
- We want points within the class close, but points between two classes far apart.



Within Class and Between Class Scatterness

$$f(\boldsymbol{x};\boldsymbol{w}) = \boldsymbol{w}^\top \boldsymbol{x}$$





μ_1 μ μ_2

Within-class Scatterness

- Embedding is $\boldsymbol{w}^{\top}\boldsymbol{x}$.
- Embedded center for class k:
  - $\hat{\mu}_k = \frac{1}{n_k}\sum_{i,y_i=k} \boldsymbol{w}^{\top}\boldsymbol{x}_i$
- Within class scatterness of class k:
- $s_{\mathrm{w},k} = \sum_{i,y_i=k}\left(\boldsymbol{w}^{\top}\boldsymbol{x}_i - \hat{\mu}_k\right)^2$
  - Sum over points in **individual** classes.

Between-class Scatterness

- Embedded dataset center:
  - $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{w}^{\top} \boldsymbol{x}_i$
- Between-class scatterness
  - $s_{\mathrm{b},k} = n_k (\hat{\mu}_k - \hat{\mu})^2$
    - n_k is needed to make $s_{\mathrm{b},k}$ at the same scale with $s_{\mathrm{w},k}$.

Fisher Discriminant Analysis

- **Maximizing** between class scatterness $\forall_k$.
- **Minimize** within class scatterness $\forall_k$.
- $\max_{\boldsymbol{w}} \boxed{\sum_k s_{\mathrm{b},k}} / \boxed{\sum_k s_{\mathrm{w},k}}$
- If $K = 2$, this has a simple solution that
- $\boldsymbol{w} := \boldsymbol{S}_{\boldsymbol{w}}^{-1}(\boldsymbol{\mu}_+ - \boldsymbol{\mu}_-)$, $\boldsymbol{S}_{\boldsymbol{w}} := \sum_{k=1}^{K} \boldsymbol{S}_k$
- $\boldsymbol{S}_k$ **is sample covariance** of class k times n_k.
- Read PRML 4.14 for its derivation

$\mu_+ \xrightarrow{w} \mu_-$

←

Fisher Discriminant Analysis

- However, FDA does not learn a decision function f.

- $f(\boldsymbol{x}; \boldsymbol{w}_{\mathrm{FDA}}) = \langle \boldsymbol{w}_{\mathrm{FDA}}, \boldsymbol{x} \rangle$ obtained by FDA cannot be directly used for making a prediction:

- In general, $f(\boldsymbol{x}; \boldsymbol{w}_{\mathrm{FDA}}) > 0$ does not mean $\boldsymbol{x}$ is predicted as positive or negative data point: FDA does not care about classification accuracy, a.k.a., minimizing FP or FN.

Probabilistic Generative Classifiers

Probabilistic Classification

- How to put classification problem under a prob. framework?

- **Minimize Expected Loss**:

$$\hat{y} \coloneqq \mathrm{argmin}_{y_0} \mathbb{E}_{p(y|\boldsymbol{x})}[L(y, y_0)\ |\boldsymbol{x}]$$

- We need: $p(y|\boldsymbol{x})$, $y \in \{1, \dots, K\}$

- Discriminative: Infer $p(y|\boldsymbol{x})$ directly.
- **Generative**: Infer $p(y|\boldsymbol{x}) \propto p(\boldsymbol{x}|y)p(y)$, infer $p(\boldsymbol{x}|y)$!

Continuous Input Variable

- To infer $p(\boldsymbol{x}|y)$, we need a model.
- If $\boldsymbol{x}$ is continuous, MVN is a natural choice for $p(\boldsymbol{x}|y)$.

- **Model** $p(\boldsymbol{x}|y = k; \boldsymbol{w}) \coloneqq N_{\boldsymbol{x}}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
- Assuming IID-ness over all $\boldsymbol{x}_i$, and shared covariance $\boldsymbol{\Sigma}$
- **Write down the likelihood** over D:
- $p(D|\boldsymbol{w}) = \prod_{i \in D} p(\boldsymbol{x}_i, y_i|\boldsymbol{w}) = \prod_{i \in D} p(\boldsymbol{x}_i|y_i; \boldsymbol{w})p(y_i)$

$$= \prod_{i \in D} N_{\boldsymbol{x}}\left(\boldsymbol{\mu}_{y_i}; \boldsymbol{\Sigma}\right) p(y_i)$$

Continuous Input Variable

- $\hat{\boldsymbol{\mu}}_{1\ldots K}, \hat{\boldsymbol{\Sigma}} \;\; := \arg \max_{\boldsymbol{\mu}_{1\ldots k}, \boldsymbol{\Sigma}} \; \sum_{i\in D} \log N_{\boldsymbol{x}}\left(\boldsymbol{\mu}_{y_i}; \boldsymbol{\Sigma}\right) p(y_i)$

1. Plug in estimates for $p(y_i)$, which is $\frac{n_k}{n}$.
2. Now work out the MLE for $\hat{\boldsymbol{\mu}}_k := \frac{1}{n_k} \sum_{i\in D, y_i=k} \boldsymbol{x}_i$
3. Plug in $\hat{\boldsymbol{\mu}}_k$ to work out

$$\hat{\boldsymbol{\Sigma}} := \sum_{k=1\ldots K} \frac{n_k}{n} \underbrace{\boxed{\frac{1}{n_k} \sum_{i\in D, y_i=k} (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)^\top}}_{\text{MLE of covariance of individual classes!}}$$

Linear Decision Boundary

- **Prove**: when using shared covariance matrix MVN model, the decision boundary is piecewise-linear.
- **Prediction**: $\hat{y} \coloneqq \operatorname{argmax}_y p(y|\boldsymbol{x};\widehat{\boldsymbol{w}}) \propto p(\boldsymbol{x}|y;\widehat{\boldsymbol{w}})p(y)$
- The decision boundary is

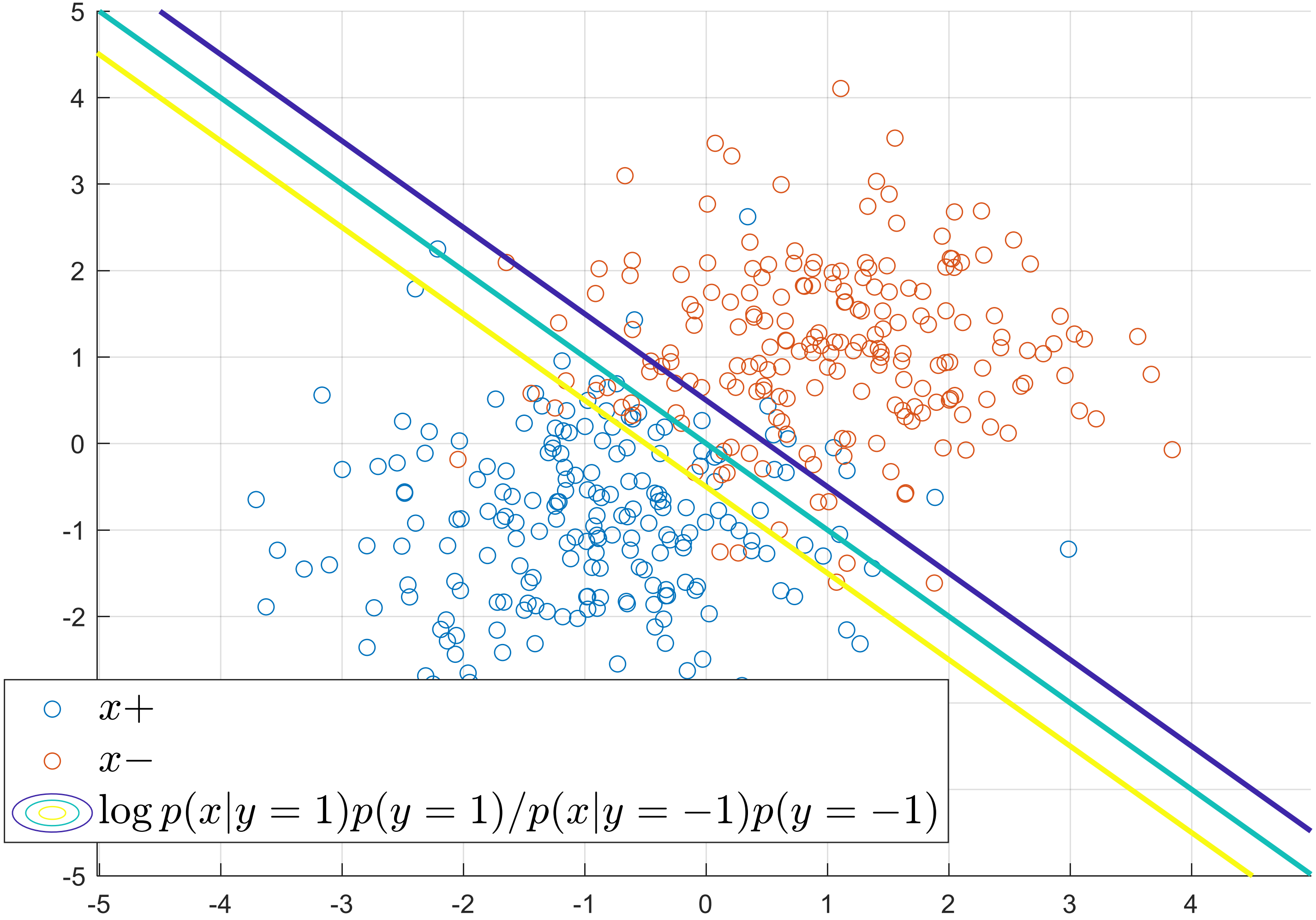
$$\{\boldsymbol{x}|p(y=k|\boldsymbol{x};\widehat{\boldsymbol{w}}) = p(y=k'|\boldsymbol{x};\widehat{\boldsymbol{w}})\}$$
$$\forall k \neq k'$$

Which is the same as the set

$$\left\{\boldsymbol{x}\middle|\frac{p(\boldsymbol{x}|y=k;\widehat{\boldsymbol{w}})p(y=k)}{p(\boldsymbol{x}|y=k';\widehat{\boldsymbol{w}})p(y=k')} = 1\right\}$$
$$\forall k \neq k'$$

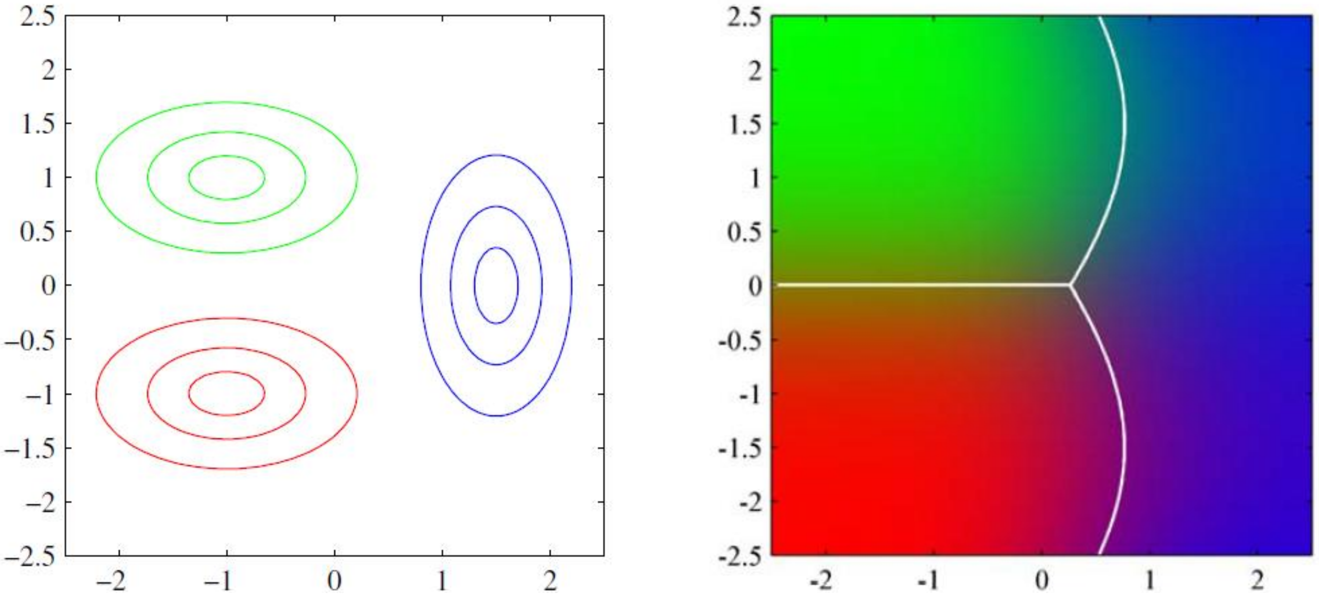
Hint: take log on both sides of the equality.

Linear Decision Boundary



Continuous Input Variable

- You can also assume for each class k, there are different covariance matrices $\boldsymbol{\Sigma}_k$.
- The MLE reduces to estimating individual $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$.
- **The decision boundary is no longer linear.**



PRML, Figure 4.11

Discrete Input Variable $\boldsymbol{x}$

- In many classification tasks, we are dealing with discrete variables as $\boldsymbol{x}$. For example, in a spam filter,
- $\boldsymbol{x} \coloneqq \left[x^{(1)}, \dots, x^{(d)}\right]^\top$ are frequencies of words in a document. This is called “bag of words” representation.
- $y \in \{\mathrm{spam}, \mathrm{ham}\}$.

- For example, the document “to be or not to be”
- $\boldsymbol{x} \coloneqq [\mathrm{to} = 2, \mathrm{be} = 2, \mathrm{or} = 1, \mathrm{not} = 1, \mathrm{question} = 0]^\top$.
- $x^{(i)} \in \{\mathrm{to}, \mathrm{be}, \mathrm{or}, \mathrm{not}, \mathrm{question}\}$

Naïve Bayes

- Assume $x^{(1)} \ldots x^{(d)}$ are conditionally independent given y
- $p(\boldsymbol{x}|y) = \prod_{i=1\ldots d} p\left(x^{(i)}\middle|y\right)$

- $p\left(x^{(i)}\middle|y = k\right)$ is the probability of word i occurs in class k.
- It is easy to estimate:

$$p\left(x^{(i)}\middle|y = k\right) \approx \frac{\sum_{j \in D, y_j = k} x_j^{(i)}}{\sum_{j \in D, y_j = k} \sum_{i=1}^{d} x_j^{(i)}}$$

- $p(\text{to}|y = \text{spam})$ is occurrences of the word “to” in “spam” emails divided by total number of words in “spam” emails in our training dataset.

Naïve Bayes

- Prediction: $\hat{y} \coloneqq \operatorname{argmax}_y p(\boldsymbol{x} = \boldsymbol{x}_0 | y) p(y)$

- $p(y = k)$: $\frac{n_k}{n}$
- $p(\boldsymbol{x} = \boldsymbol{x}_0 | y)$: $\prod_{i=1\ldots d} p\left(x^{(i)} \middle| y\right)^{x_0^{(i)}}$
  - $p\left(x^{(i)} \middle| y\right)$ has been obtained by previous counting.
  - Power $x_0^{(i)}$ is used assuming occur. of words are independent.
- $p(\boldsymbol{x} = \text{"}\boldsymbol{to\ be\ or\ not\ to\ be}\text{"} | y)$:

$$p(to|y)^2 p(be|y)^2 p(or|y) p(not|y)$$

Conclusion

- We have studied classification problem:

- Geometry of decision function
- Least square classifier
- Fisher discriminant analysis
  - Within and between scatterness

- Generative Classifiers:
  - MVN for continuous input variable
  - Naïve Bayes for discrete input variable

Homework

- Prove the statement on page 32.

- Put Naïve Bayes under an MLE framework.
- **Hint:** Assume $p(\boldsymbol{x}|\pi_{1\dots d})$ is a multinomial distribution with event probabilities $\pi_{1\dots d}$.
- $\frac{x^{(i)}}{\sum_{i=1}^{d} x^{(i)}}$ is the MLE of π_i given $D = \{\boldsymbol{x}\} = \left\{\left[x^{(1)} \dots x^{(d)}\right]\right\}$

Computing Lab

- Implement a version of Perception classifier: “Simplitron”

- Demo.