CS 559 Machine Learning

Lecture 3: Linear Classification

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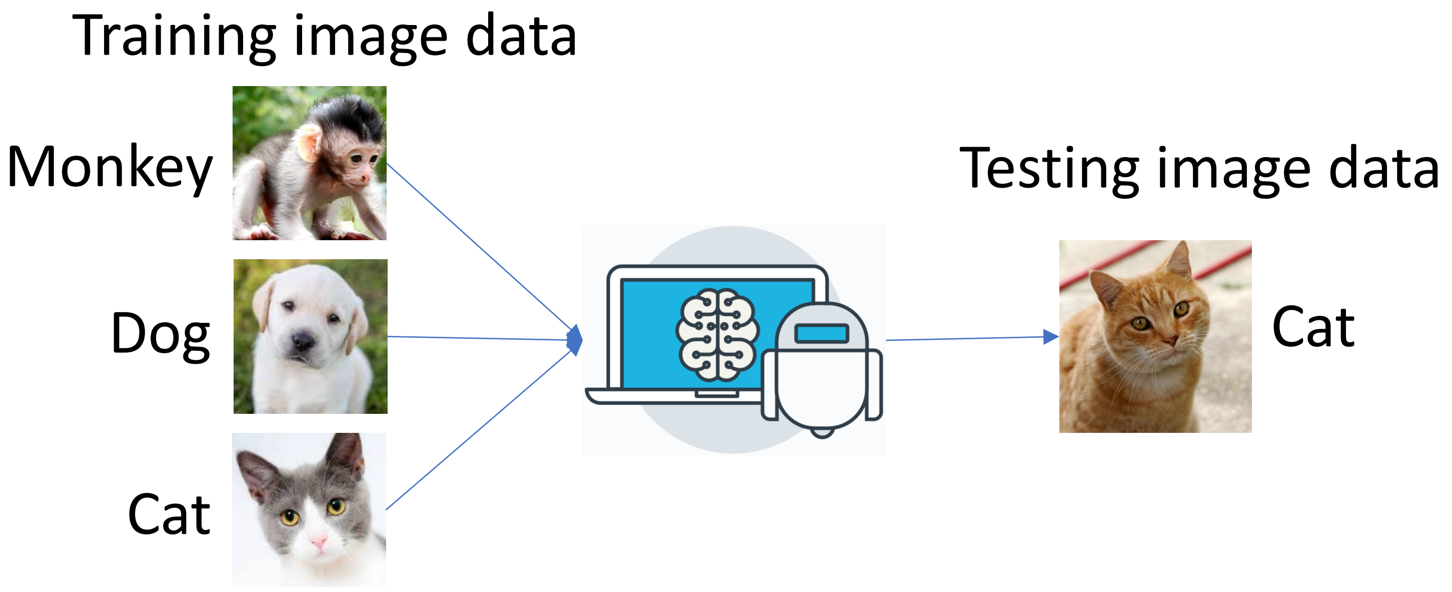
Today's Lecture

- Generative vs Discriminative Classification
- Linear Discriminant Analysis
- Least Square Classification
- Fisher's Linear Discriminant
- The Perceptron Algorithm

Classification Task

- Task: find a function f that classifies examples into a given set of discrete classes $\{C_1, C_2, \dots, C_k\}$.



Features/Attributes (x) $\longrightarrow$ Function f $\longrightarrow$ $y \in \{C_1, C_2, \dots, C_k\}$

Linear Classification

- Decision boundaries/surfaces: divide the input space into decision regions.
- For linear classification, the decision boundaries are linear functions of the input x.
- Linear separable: datasets that can be exactly separated by linear decision boundaries are linear separable.

Generative and Discriminative Approach

Decision Theory for Classification

- Decision theory, combined with probability theory, allows us to make optimal decisions in situations involving uncertainty.
  - Training data: input values X and target values y
  - Learning stage: use the training data to learn a model for $p(C_k|x)$, where C_k represents the class k.
  - Decision stage: use the learnt posterior probabilities to make optimal class assignments.

Generative Methods

- Solve the inference problem by estimating the class-conditional density $p(x|C_k)$ for each class C_k
- Estimate the class prior probability $p(C_k)$
- Use Bayes' theorem to get the class posterior probability:

$$p(C_k|x) = \frac{p(x|C_k)p(C_k)}{p(x)}$$

where $\quad p(x) = \sum_{k=1}^{K} p(x|C_k)p(C_k)$

- Use decision theory to determine class label for each new input x.

Discriminative Methods

- Directly solve the inference problem of estimating the class posterior probabilities $p(C_k|x)$.

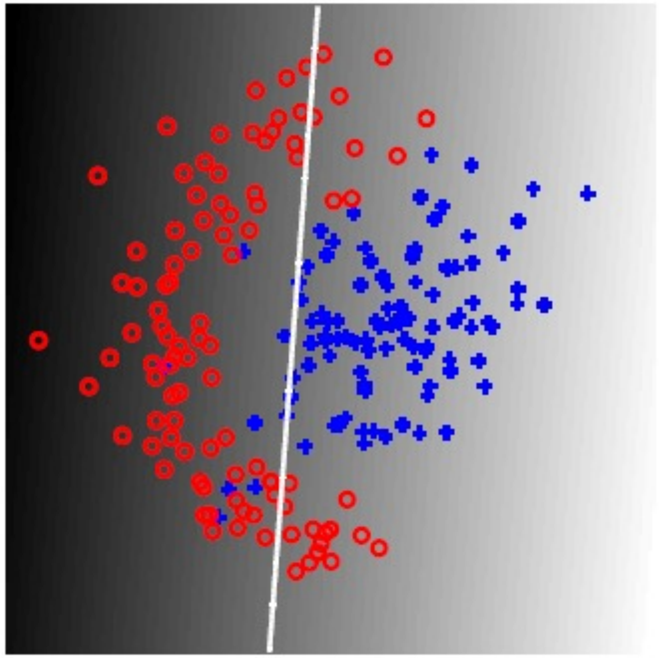
- Discriminative Functions: Find a function $f(x)$ which maps each input directly onto a class label. Probabilities play no role here.

- Use decision theory to determine class label for each new input x.

Linear Discriminant Function

Binary Classification

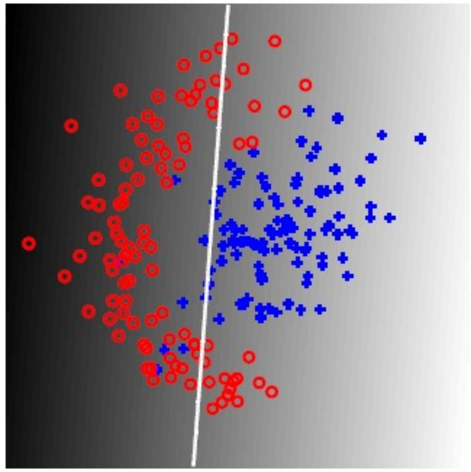
- Task: Assign each data point to one of two classes (e.g., 0/1, 1/-1).
- Examples:
  - Is there a face in this image?
  - Is this email spam or not?
  - Based on this brain-scan, does this patient have a given disease or not?
  - Will this customer buy this product or not?
  - Will this patient be re-hospitalized or not?

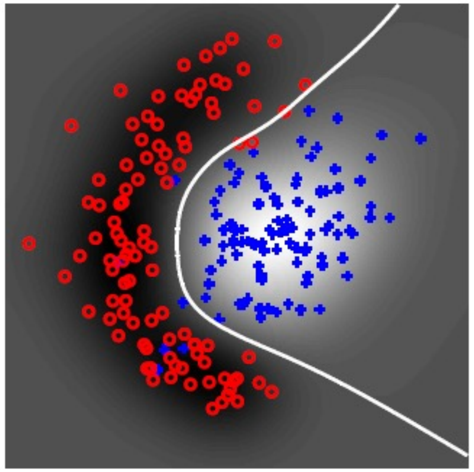


- Notation: $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$, with $y_n = 1$ if x_n belongs to class 1, and $y_n = -1$ if x_n belongs to class -1.

Linear Discriminant Function

- Discriminative methods learn the class posterior $p(C_k|x)$.
- The simple way would be the linear discriminant function.
- The discriminant function directly assigns the class label for each input vector x.
- Linear algorithms can be used together with nonlinear feature spaces or nonlinear basis functions to solve nonlinear classification problems!





Linear Discriminant Function

- Linear discriminants separate the space by a hyperplane, and the parameters define its normal vector.
- Decision function: $f(x) = w^T x + w_0$, where w represents the weight vector, and w_0 is the bias that determines the location of the decision boundary.
- Classification task:

$$\text{If } f(x) \geq 0,\ x \rightarrow \text{class } 1$$

$$\text{If } f(x) < 0,\ x \rightarrow \text{class } -1$$

- The decision boundary is defined by equation $f(x) = 0$, which is a hyperplane.

Geometrical Properties

- Decision boundary: $f(x) = w^T x + w_0 = 0$
- Let x_1, x_2 be two points which lie on the decision boundary

$$f(x_1) = w^T x_1 + w_0 = 0$$
$$f(x_2) = w^T x_2 + w_0 = 0$$
$$w^T(x_1 - x_2) = 0$$

- Therefore, w represents the orthogonal direction to the decision boundary. It is the normal vector to the hyperplane, and points into the positive class or negative class.

Sign is Important!

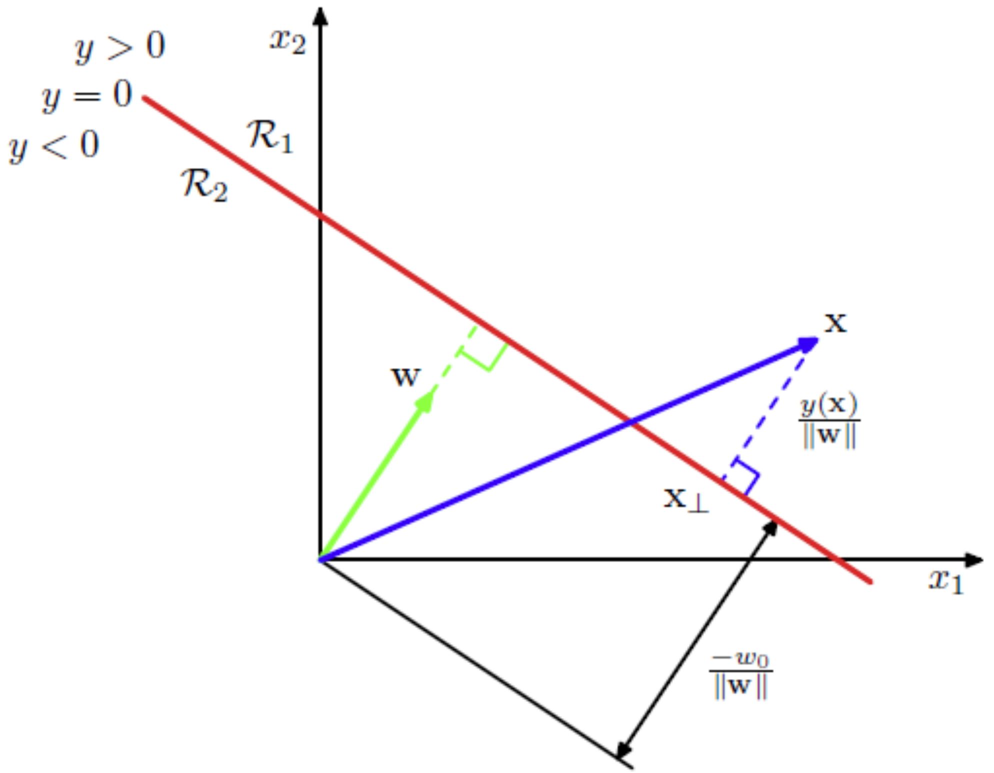
- We can observe that the sign of $f(x)$ is important for classification.
- The scale of the weight w does not matter.
- Therefore, we can use the normalized weight w with length $\|w\| = 1$.

Geometrical Properties Cont.

- $w^{*T} = \frac{w^T}{\|w\|}$
- $w^{*T}(x - x_0)$ is the projection of $(x - x_0)$ onto the direction of w^*; x_0 is a point on the decision boundary.
- Thus

$$\frac{w^T}{\|w\|}(x - x_0) = \frac{1}{\|w\|}(w^T x - w^T x_0)$$
$$= \frac{1}{\|w\|}(w^T x + \omega_0) = \frac{f(x)}{\|w\|}$$

- When $x = 0$, $\frac{f(x)}{\|w\|} = \frac{\omega_0}{\|w\|}$

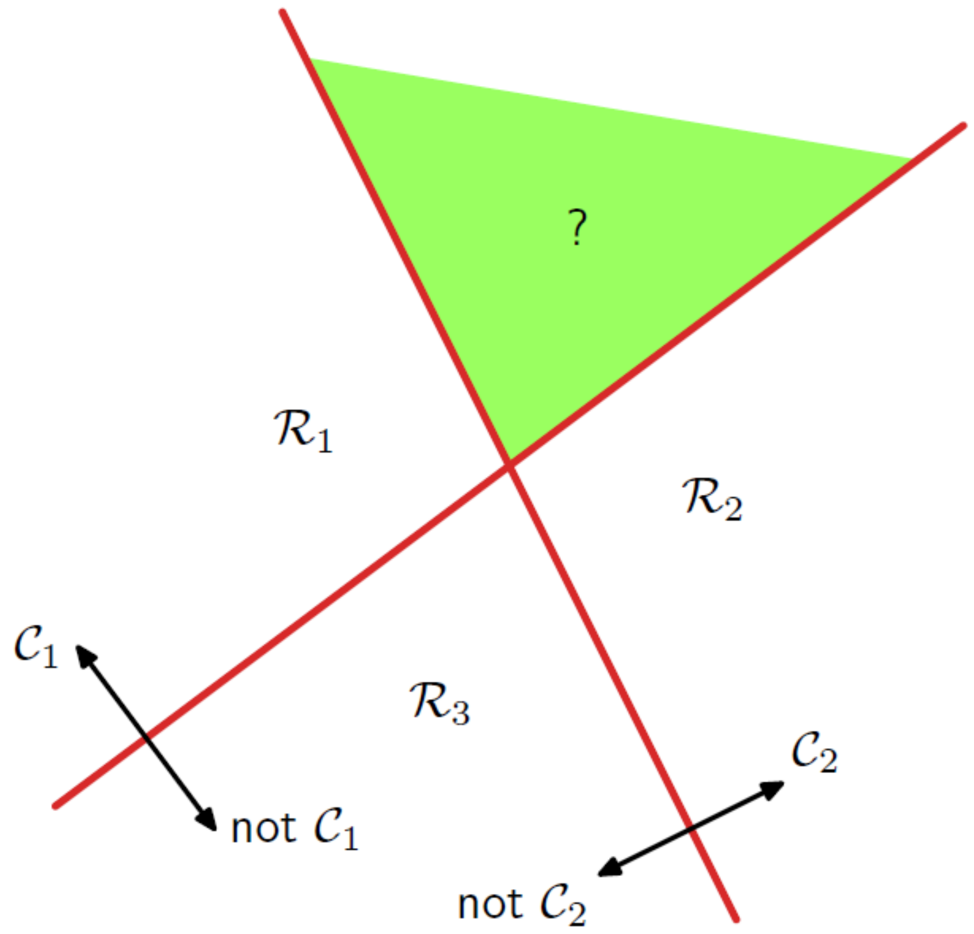


Signed orthogonal distance of the origin from the decision surface

Linear Discriminant Functions: Multiple Classes

one-versus-the-rest:

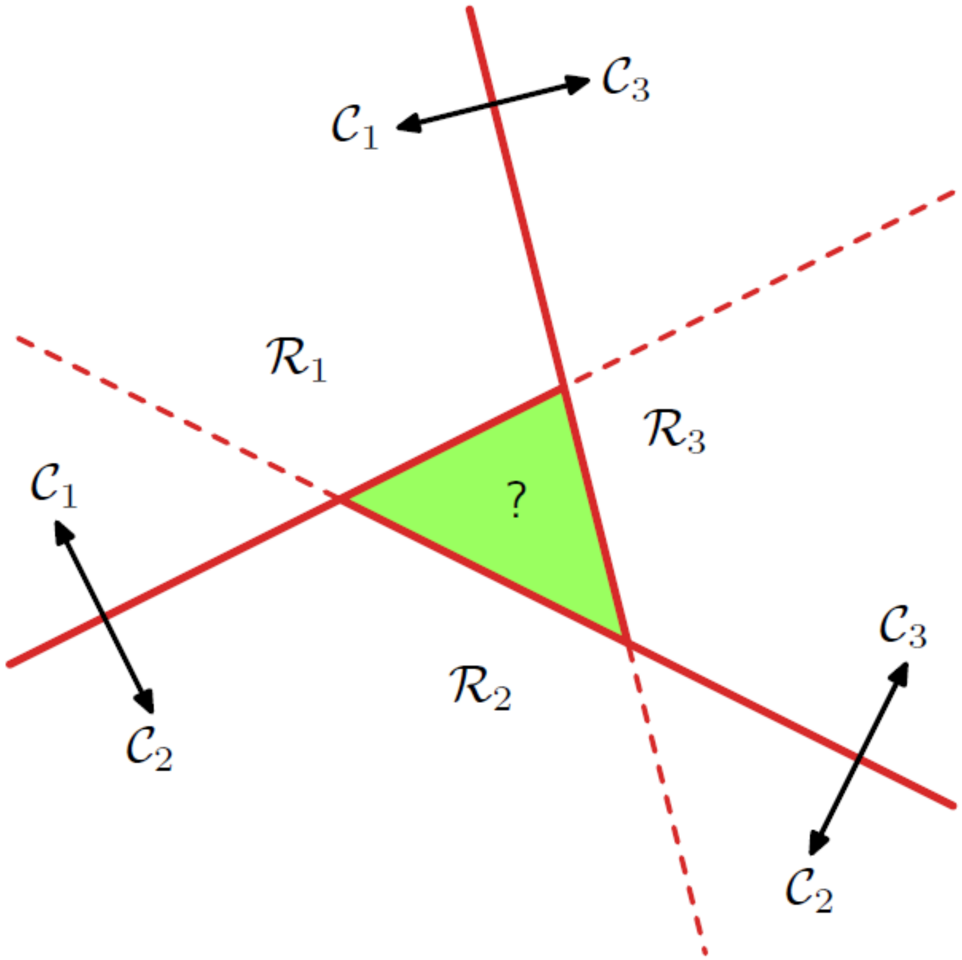
- $K - 1$ classifiers, each of which solves a two-class problem of separating points in a particular class C_k from points not in that class.
- Leads to regions of input space that are ambiguously classified, shown in green.



Linear Discriminant Functions: Multiple classes

one-versus-one:

- $\frac{K(K-1)}{2}$ classifiers, one for every possible pair of classes
- Each point is classified by majority voting amongst the discriminant functions.
- Also leads to regions of input space that are ambiguously classified , shown in green.

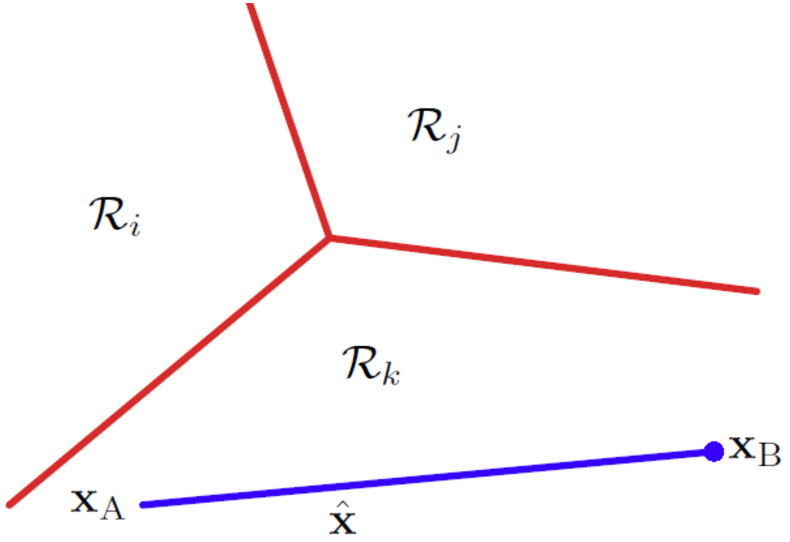


Linear Discriminant Functions: Multiple classes

- Solution: Consider a single K-class discriminant comprising K linear functions of the form
$$f_k(x) = w_k^T x + w_{k0}$$
- Assign a point x to class C_k if
$$f_k(x) > f_j(x) \; \forall j \neq k.$$
- The decision boundary between class C_k and class C_j is given by:
$$f_k(x) = f_j(x)$$

A hyperplane: $\Rightarrow \left(w_k - w_j\right)^T x + \left(w_{k0} - w_{j0}\right) = 0$

Decision boundaries



If two points lie in the same decision region, then any point on the line segment must lie in the same region.

Linear Classification Algorithms

- Mis-classification rate $C(w) = \frac{1}{N}\sum_n \delta[f(x_n) = y_n]$ (i.e. average number of errors) is difficult to optimize over w, and might have multiple solutions.
- Many algorithms can be derived by replacing C by another cost-function which can be optimized.
  - Least-square Classification
  - Fisher's Linear Discriminant
  - The Perceptron Algorithm
  - Logistic Regression
  - Support Vector Machines

Least Square Classification

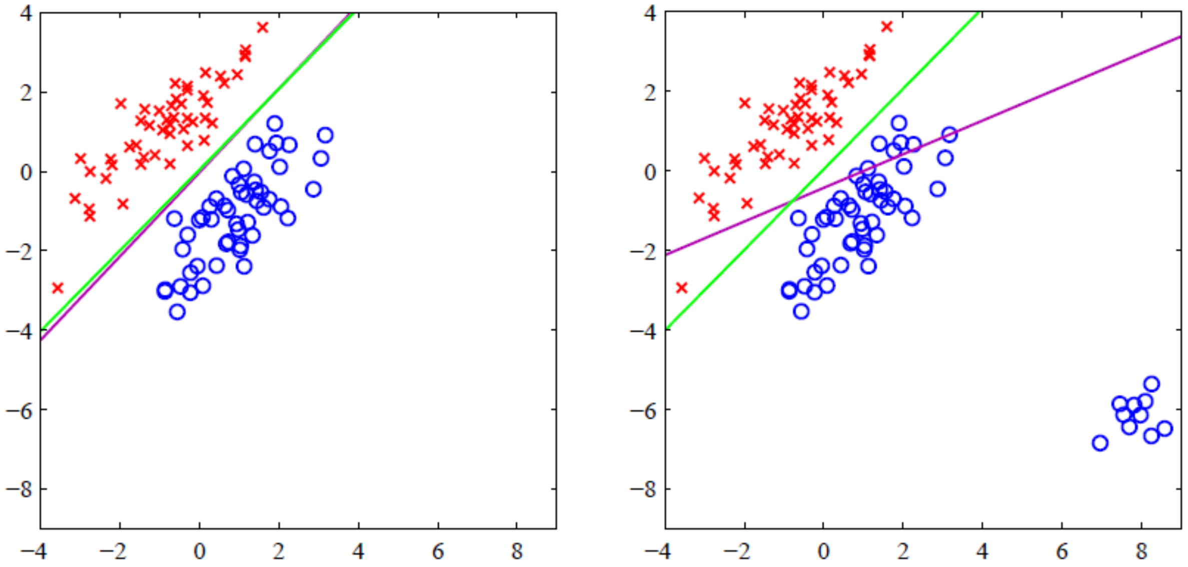
Least Square Classification

- We have to fit the function $f(x) = xw^T + \omega_0$ to data.
- Simply do a linear regression from x to y by minimizing the sum-of-squared errors $\sum_n (f(x_n) - y_n)^2$.
- $w_{reg} = (\sum_n x_n x_n^T)^{-1} \sum_n x_n y_n$

- Questions: what is the limitation of Least Square Classification?

Least Square Classification

- Least squares solutions lack robustness to outliers.
- The decision boundary changed significantly when extra data points are added.

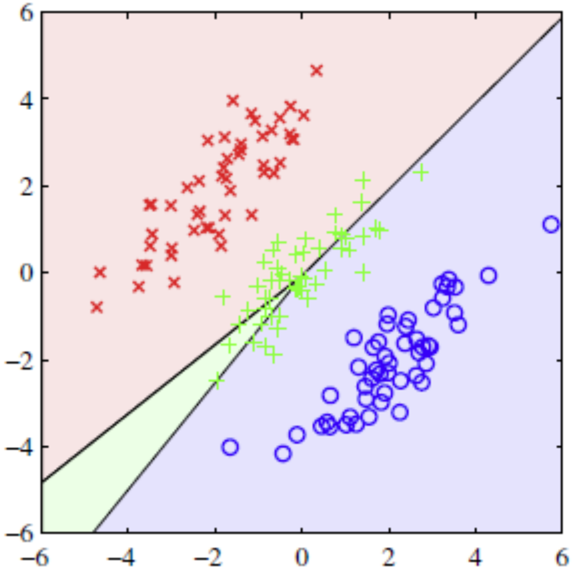


Bishop PRML Figure 4.4.

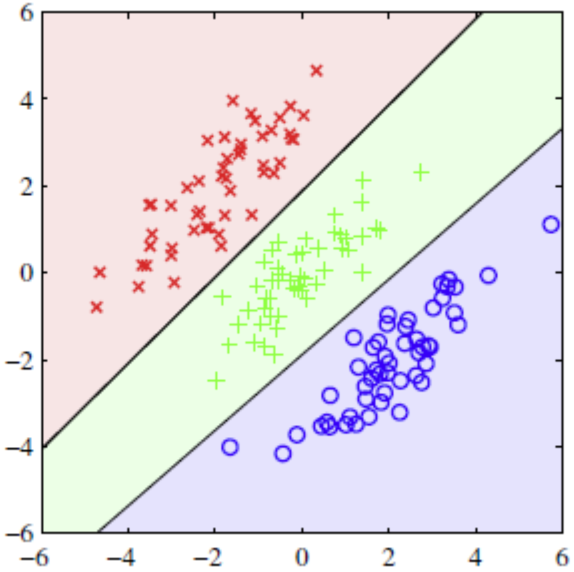
Purple: least squares. Green: logistic regression

Least Square Classification

- Example of a synthetic data set with three classes. Most of the points in the green class are misclassified.
- The background colors denote the respective classes of the decision regions.



Least square discriminant



Logistic regression

Bishop PRML Figure 4.5

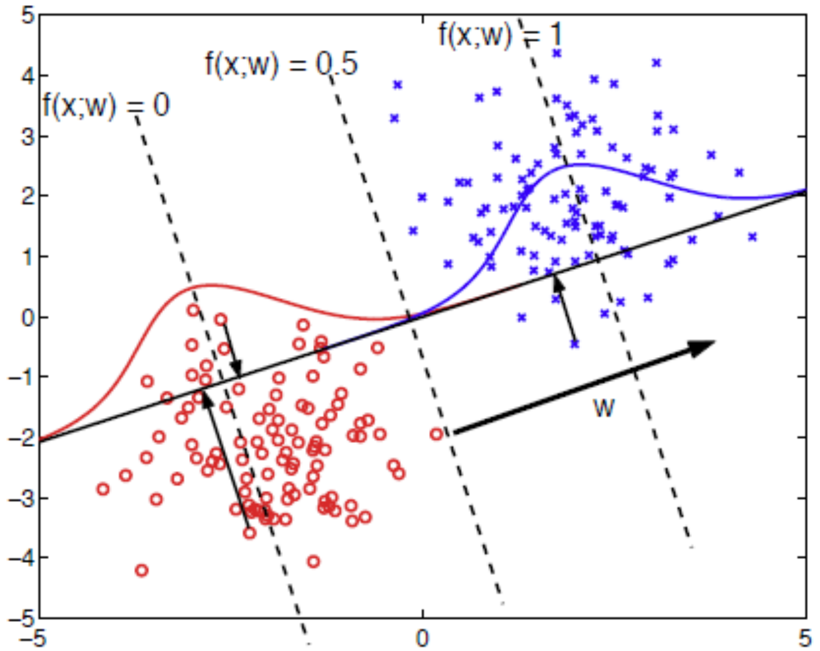
Fisher’s Linear Discriminant

Classification via Projection

- A linear function: $f(x) = w^T x + w_0$ assuming in 2D, projects each point x to a line parallel to w:

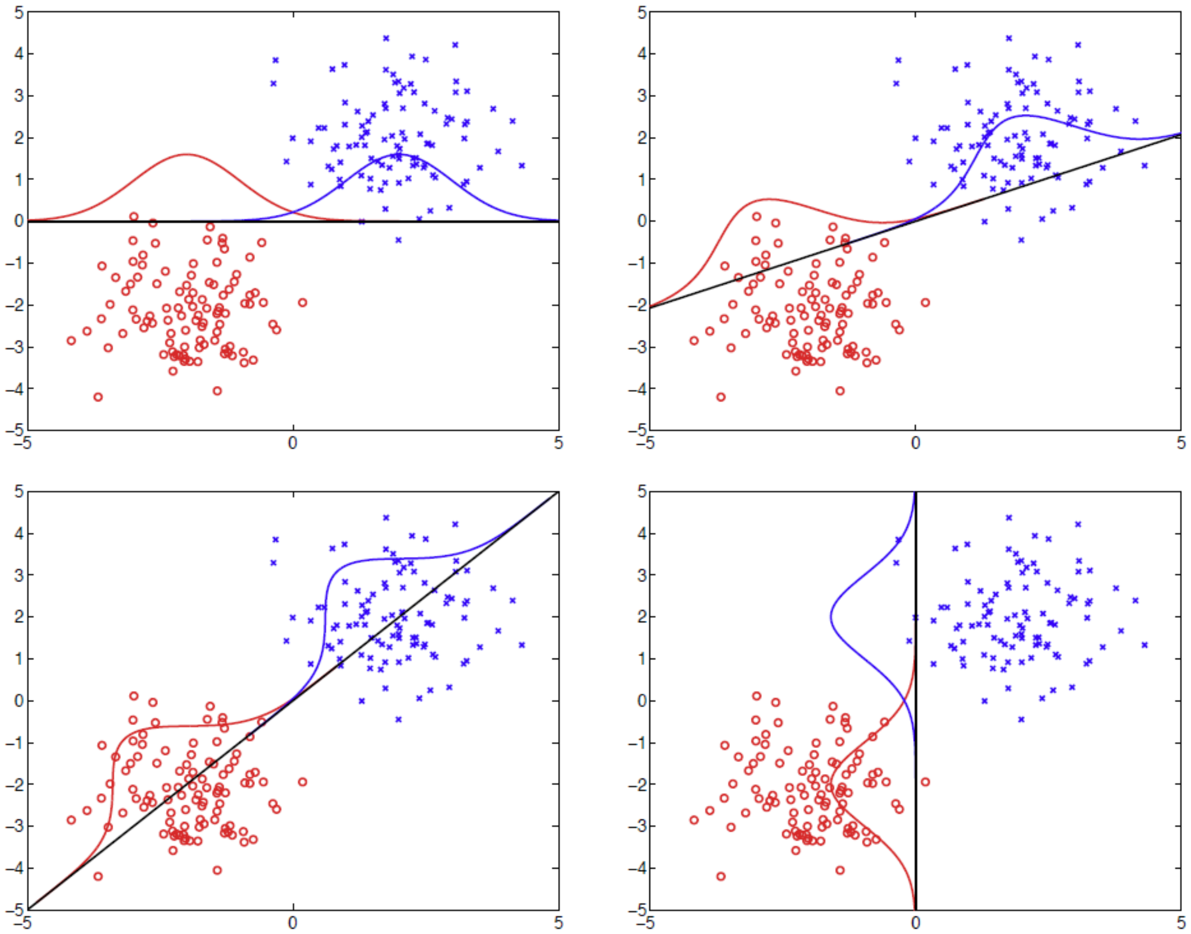
$$x_1 \rightarrow z_1 = w^T x_1$$
$$x_2 \rightarrow z_2 = w^T x_2$$
$$\dots$$
$$x_N \rightarrow z_N = w^T x_N$$

- We can study how well the projected points $z_1, \dots, z_N$ (viewed as functions of w) are separated across the classes.



Classification via Projection

- By varying w we get different levels of separation between the projected points.
- Find w that maximizes the separation of the projected points across classes.
- Quantify the separation (overlap) in terms of means and variances of the resulting 1-dimensional class distributions.



Fisher's Linear Discriminant

- One way to view a linear classification model is in terms of dimensionality reduction.
- For binary classification, suppose we project x onto one dimensional:

$$f = w^T x$$

- A threshold t can be set to assign the label for x:

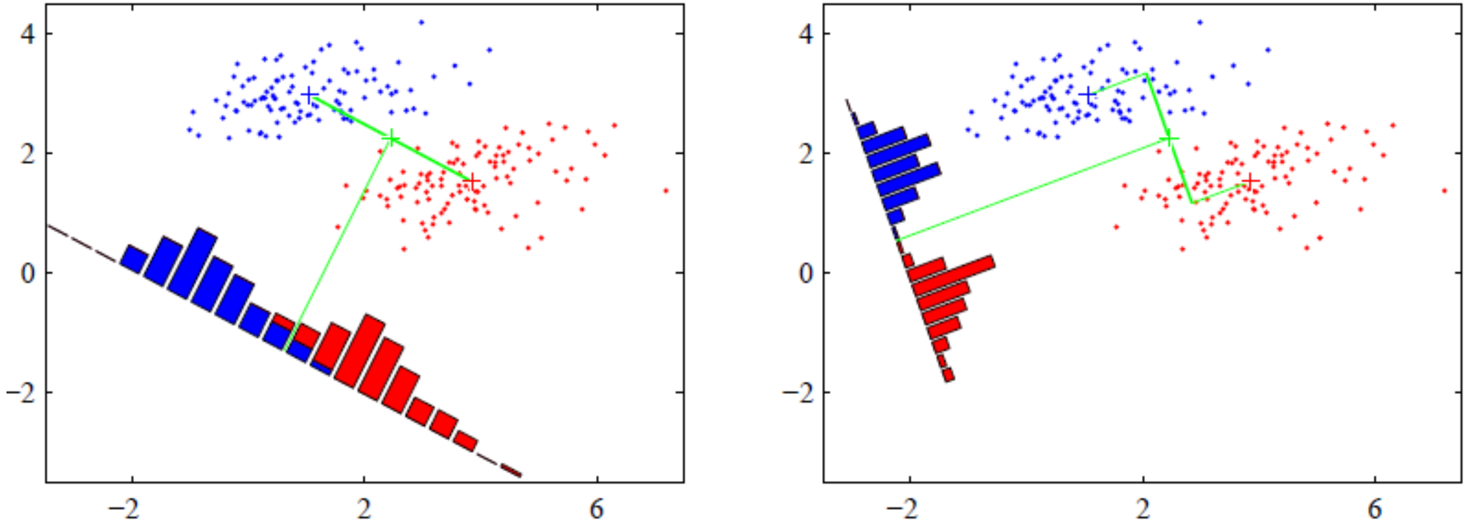
$$\text{If } f \leq t, x \rightarrow C_1$$

$$\text{If } f > t, x \rightarrow C_2$$

- In general, the projection leads to considerable loss of information, and classes well separated in the original space may strongly overlap in one dimension.

Fisher's Linear Discriminant

- Find a direction along which the projected samples are well separated.
- This is exactly the goal of linear discriminant analysis (LDA).
- In other words: we want to find the linear projection that best separates the data, i.e. best discriminates data of different classes.



Fisher's Linear Discriminant

- We use N_1 and N_2 to represent the number of samples for class C_1 and C_2, respectively.
- Consider the normalized weight vector w with $||w|| = 1$.
- Then, $w^T x$ is the projection of x onto the direction of w.
- Objective: find the projections of $w^T x$ so that $x \in C_1$ and $x \in C_2$ can be well separated (maximize the class separation).

How to Measure the Separation?

An intuitive measure of the separation between the projected points is the difference of the sample means.

- Sample mean vector of class C_1:

$$m_1 = \frac{1}{N_1} \sum_{x \in C_1} x$$

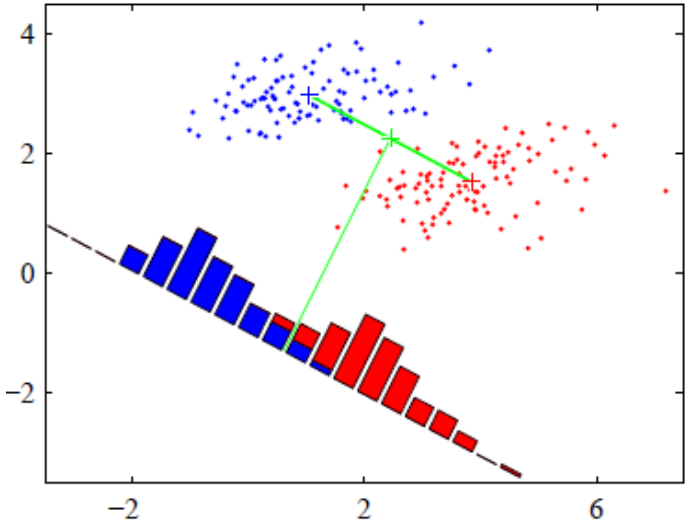
- Sample mean vector of class C_1 after projection:

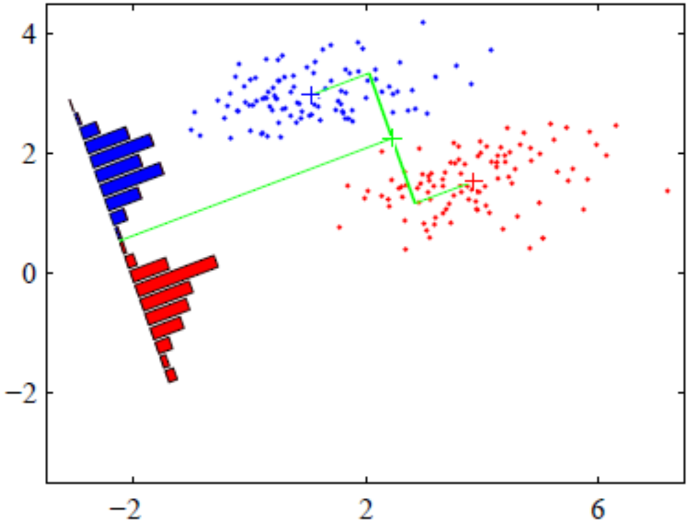
$$m_1' = \frac{1}{N_1} \sum_{x \in C_1} w^T x = w^T m_1$$

- Objective is to choose w that can maximize the separation $|m_1' - m_2'| = w^T |m_1 - m_2|$

How to Measure the Separation?

- Choose w that maximizes projection-distance of class means $|m_1' - m_2'| = w^T|m_1 - m_2|$
- Limitation: maximizing distance between means, but the projected variances within each class might be large (large class overlap).





How to Measure the Separation?

- To obtain good separation of the projected data, we really want the difference between the means to be large relative to some measure of the standard deviation of each class.
- Variance of the projected samples of class C_1:

$$s_1^2 = \sum_{x \in C_1} (w^T x - m_1')^2$$

- Total within-class variance of the projected samples will be:

$$s_1^2 + s_2^2$$

- Fisher linear discriminant analysis: Fisher criterion defined by the ratio of the between-class variance to the within-class variance.

$$\arg\max_w \frac{|m_1' - m_2'|^2}{s_1^2 + s_2^2}$$

Fisher's Linear Discriminant

- Define $J(w) = \frac{|m_1' - m_2'|^2}{s_1^2 + s_2^2}$. To obtain $J(w)$ as an explicit function of w, we define the following matrices:

$$S_1 = \sum_{x \in C_1} (x - m_1)(x - m_1)^T$$

- Within-class covariance matrix: $S_W = S_1 + S_2$
- Then

$$s_1^2 = \sum_{x \in C_1} (w^T x - m_1')^2 = \sum_{x \in C_1} (w^T x - w^T m_1)^2$$

$$= \sum_{x \in C_1} w^T (x - m_1)(x - m_1)^T w = w^T S_1 w$$

Fisher's Linear Discriminant

- Therefore, $s_1^2 = w^T S_1 w$ and $s_2^2 = w^T S_2 w$.
- Further:

$$s_1^2 + s_2^2 = w^T S_1 w + w^T S_2 w = w^T (S_1 + S_2) w = w^T S_W w$$

- Similarly:

$$\begin{aligned} |m_1' - m_2'|^2 &= (w^T m_1 - w^T m_2)^2 \\ &= w^T (m_1 - m_2)(m_1 - m_2)^T w \\ &= w^T S_B w \end{aligned}$$

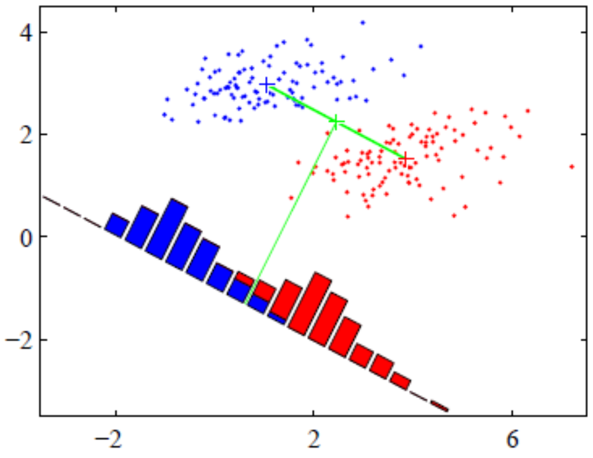
- Where $S_B = (m_1 - m_2)(m_1 - m_2)^T$ is the between-class covariance matrix.

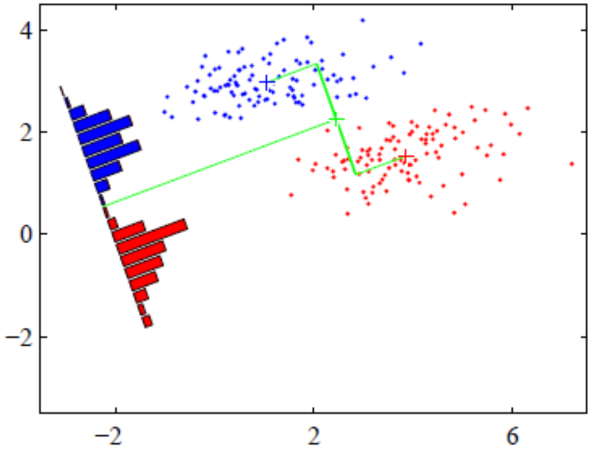
Fisher's Linear Discriminant

- Therefore, $J(w) = \frac{\left|m_1' - m_2'\right|^2}{s_1^2 + s_2^2} = \frac{w^T S_B w}{w^T S_W w}$
- Differentiating with respect to w, $J(w)$ is maximized when
$$(w^T S_B w) S_W w = (w^T S_W w) S_B w$$
- We can observe that $S_B w = (m_1 - m_2)(m_1 - m_2)^T w$ always in the direction of $(m_1 - m_2)$ since $(m_1 - m_2)^T w$ is a scalar.
- Also, we only care about the direction of w, so we can drop the scaler factors $(w^T S_B w)$ and $(w^T S_W w)$.
- Therefore, we have the solution:
$$w \propto S_W^{-1}(m_1 - m_2)$$

Summary of Fisher's Linear Discriminant

- $m_1 = \frac{1}{N_1} \sum_{x \in C_1} x$, $m_2 = \frac{1}{N_2} \sum_{x \in C_2} x$
- Separation: Maximize projection-distance of class means
- But the projected variances within each class might be large
- Fix: Maximize the ratio of between-class variance to within-class variance ("signal to noise").
- Fisher criterion $J(w) = \frac{|m_1' - m_2'|^2}{s_1^2 + s_2^2}$
- Solution: $w \propto S_W^{-1}(m_1 - m_2)$





Fisher’s Linear Discriminant

- Gives the linear function with the maximum ratio of between-class variance to within-class variance.
- LDA is a linear technique for dimensionality reduction. The classification problem has been reduced from a d-dimensional problem to a more manageable one-dimensional problem.
- Note that LDA uses class labels.
- The analysis can be extended to multiple classes or non-linear problems.
- More details can be found in Bishop PRML Section 4.1.6

The Perceptron Algorithm

The Perceptron Algorithm

- First learning algorithm for neural networks. (Frank Rosenblatt, 1957)
- Originally introduced for character classification, where each character is represented as an image.
- It is a type of linear classifier that makes predictions based on a linear predictor function and a set of weights with the input feature vector.

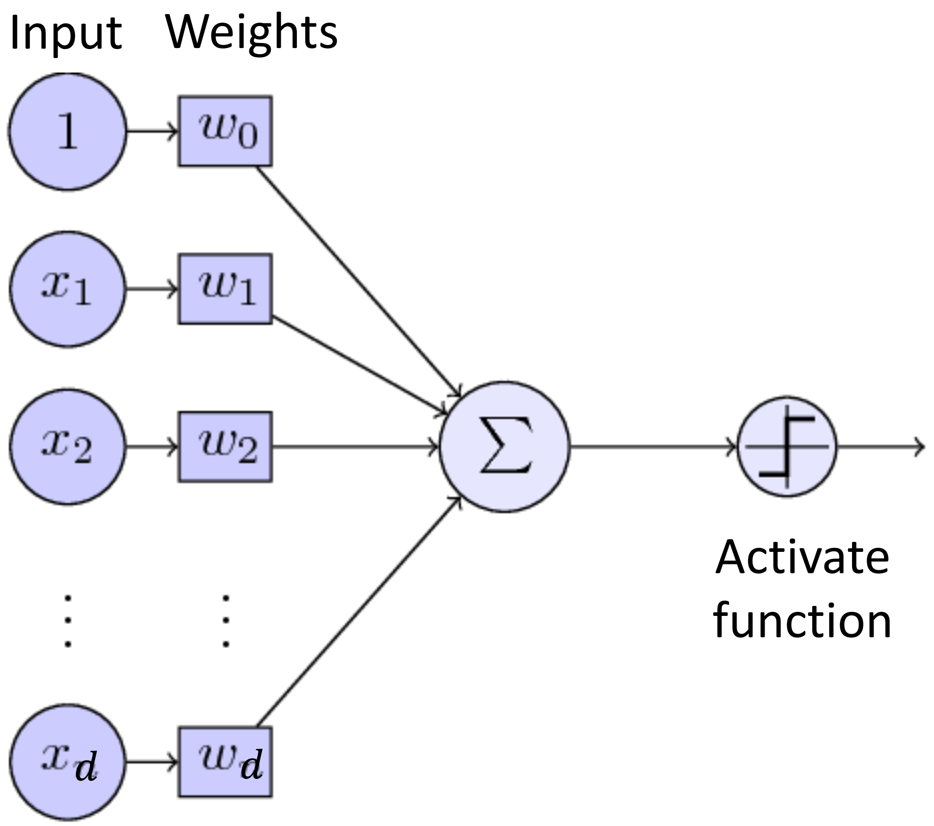
The Perceptron Algorithm

- Total input to output node:

$$\sum_j w_j x_j$$

- Output unit performs the function (activation function):

$$H(x) = \begin{cases} 1 \;\; if \;\; x \geq 0 \\ 0 \;\; if \;\; x < 0 \end{cases}$$



Perceptron: Learning Task

- Goal: compute a mapping from inputs to the outputs.
- Example: two-class character recognition problem.
  - Training set: a set of images representing either the character ‘a’ or the character ‘b' (supervised learning);
  - Learning task: learn the weights so that when a new unlabeled image comes in, the network can predict its label.
  - Setting: d input units (intensity level of a pixel), 1 output unit.

Perceptron: Learning Algorithm

- The algorithm proceeds as follows:
  - Initial random setting of weights;
  - The input is a random sequence $\{x_k\}$
  - For each element of class C_1, if output = 1 (correct), do nothing; otherwise, update weights.
  - For each element of class C_2, if output = 0 (correct), do nothing; otherwise, update weights.

Perceptron: Learning Algorithm

- More formally:
  - $x = (x_1, x_2, \dots, x_d)^T$
  - $w = (w_1, w_2, \dots, w_d)^T$
- Output: $w^T x = w_1 x_1 + w_2 x_2 + \cdots + w_d x_d$
- Output class 1 if $w^T x \geq 0$, otherwise, output class 0.

Perceptron: Learning Algorithm

- The objective is to learn the weights so that the perceptron can correctly discriminate elements of C_1 from elements of C_2
- Given x in input, if x is classified correctly, weights are unchanged, otherwise:

$$w = \begin{cases} w + x \ \ if\ an\ element\ of\ class\ C_1\ was\ classified\ as\ in\ C_2 \\ w - x \ \ if\ an\ element\ of\ class\ C_2\ was\ classified\ as\ in\ C_1 \end{cases}$$

Perceptron: Learning Algorithm

- It is online:
  - Only process one example at a time, instead of considering the entire dataset at the same time.
- Error-Driven Updating:
  - If it is doing well, it doesn't update the parameters.
  - Only when the prediction is incorrect, it updates the parameters.
  - The parameters are updated in a way that it would do better on this example next time around.
  - How to verify? Two cases.

Perceptron: Learning Algorithm

- **1^{st} case:** $x \in C_1$, but was classified in C_2. In other words, the correct answer is 1, which corresponds to $w^T x \geq 0$, but the model provides $w^T x < 0$. In the next round after updating the parameters to w'^T, we want to get closer to the correct answer (be greater):
$$w^T x < w'^T x$$
- Verify if it would do better after updating w as $w' = w + x$.
$$\begin{aligned} w'^T x &= (w + x)^T x \\ &= w^T x + x^T x \\ &= w^T x + ||x||^2 \end{aligned}$$
- Since $||x||^2 > 0$, the condition is verified.

Perceptron: Learning Algorithm

- **2^{nd} case:** $x \in C_2$, but was classified in C_1. In other words, the correct answer is 0, which corresponds to $w^T x < 0$, but the model provides $w^T x \geq 0$. In the next round after updating the parameters to w'^T, we want to get closer to the correct answer (be smaller):

$$w^T x > w'^T x$$

- Verify if it would do better after updating w as $w' = w - x$.

$$\begin{aligned} w'^T x &= (w - x)^T x \\ &= w^T x - x^T x \\ &= w^T x - ||x||^2 \end{aligned}$$

- Since $||x||^2 > 0$, the condition is verified.

The Perceptron Algorithm: Example

Example:

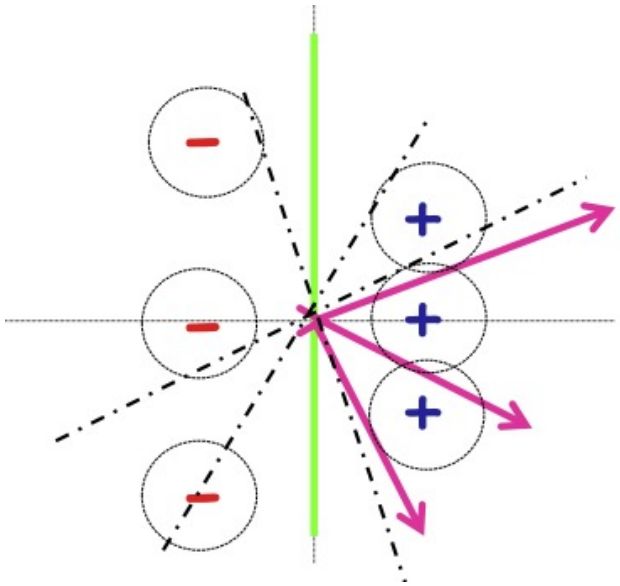
$(-1,2)$	$-$	✗
$(1,0)$	$+$	✓
$(1,1)$	$+$	✗
$(-1,0)$	$-$	✓
$(-1,-2)$	$-$	✗
$(1,-1)$	$+$	✓

$$w_1 = (0,0)$$

$$w_2 = w_1 - (-1,2) = (1,-2)$$

$$w_3 = w_2 + (1,1) = (2,-1)$$

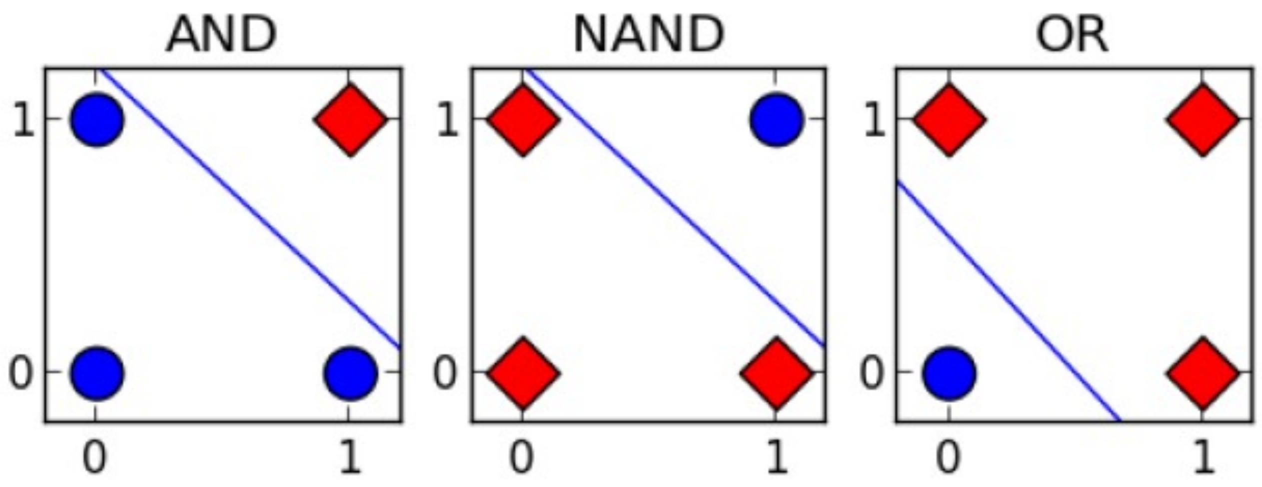
$$w_4 = w_3 - (-1,-2) = (3,1)$$



Example from: http://www.cs.cmu.edu/~mgormley/courses/606-607-f18/slides607/lecture4-pmb.pdf

Representational Power of Perceptrons

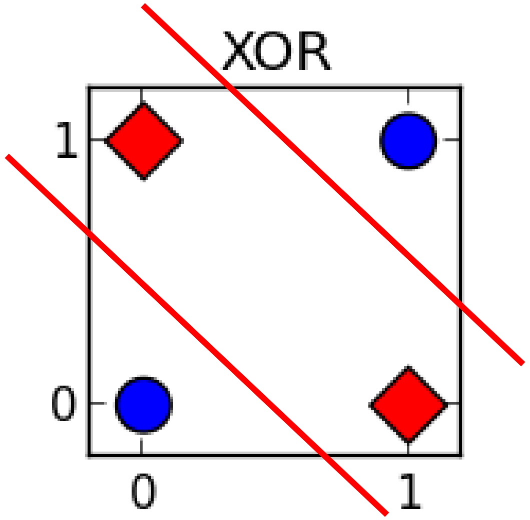
- Marvin Minsky and Seymour Papert, “Perceptrons" 1969: The perceptron can only solve problems with linearly separable classes.
  - The functions can be drawn in 2-dim graph and a single straight line separates values in two parts.
- Examples of linearly separable Boolean functions:



Representational Power of Perceptrons

- The perceptron cannot model the non-linearly separable functions: Logical XOR function (computes the logical exclusive).
  - Input: Two input arguments with values in {0,1}.
  - Output: 1 if and only if two inputs have different values.
  - For such functions, we have to use multi-layer feed-forward network.

X_1	X_2	Y
0	0	0
0	1	1
1	0	1
1	1	0



Summary of The Perceptron Algorithm

- For a random sequence $x_1, x_2, \dots, x_k$, with $x_i (i = 1, \dots, k) \in C_1 \ or \ C_2$
- For each x, if it is correctly classified, then $w_{k+1} = w_k$, otherwise,

$$w_{k+1} = \begin{cases} w_k + x \ \ if \ x \in C_1 \\ w_k - x \ \ if \ x \in C_2 \end{cases}$$

- Convergence theorem: regardless of the initial choice of weights, if the two classes are linearly separable, there exists w such that:

$$\begin{cases} w^T x \geq 0 \ \ if \ x \in C_1 \\ w^T x < 0 \ \ if \ x \in C_2 \end{cases}$$

- The learning rule will find such solution after a finite number of steps.

Summary of Today’s Lecture

- Generative vs Discriminative Classification
- Linear Discriminant Analysis
- Least Square Classification
- Fisher's Linear Discriminant
- The Perceptron Algorithm