Introduction to Machine Learning

Linear Models for Classification

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Some slides are modified from Prof. Sheng-Jyh Wang and Prof. Hwang-Tzong Chen

Classification problem

- The goal in classification is to take an input vector $\mathbf{x}$ and to assign it to one of K discrete classes C_k where $k = 1, 2, \ldots, K$.
- The input space is divided into decision regions whose boundaries are called decision boundaries or decision surfaces

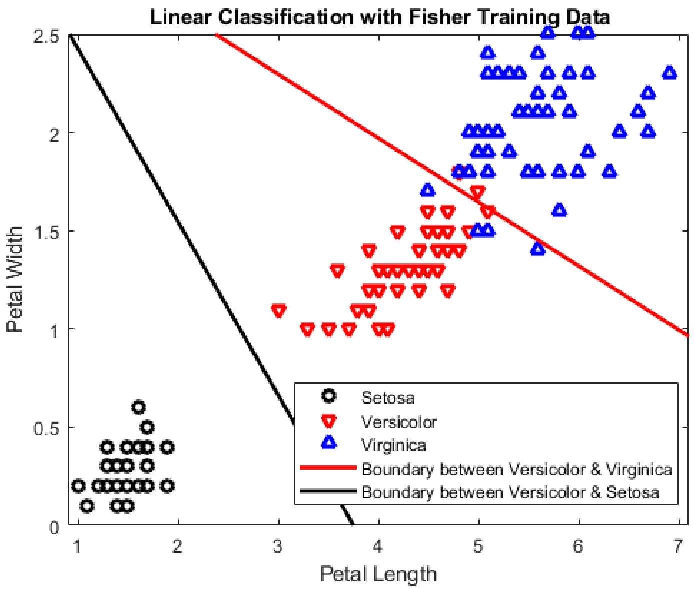
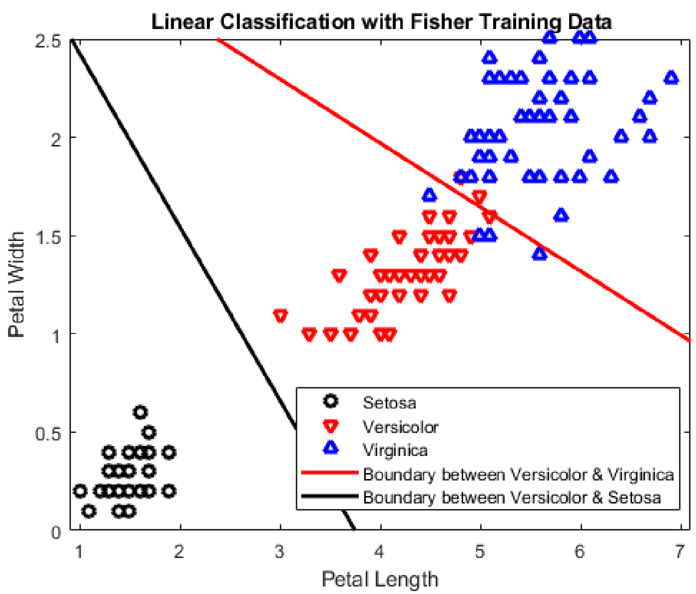


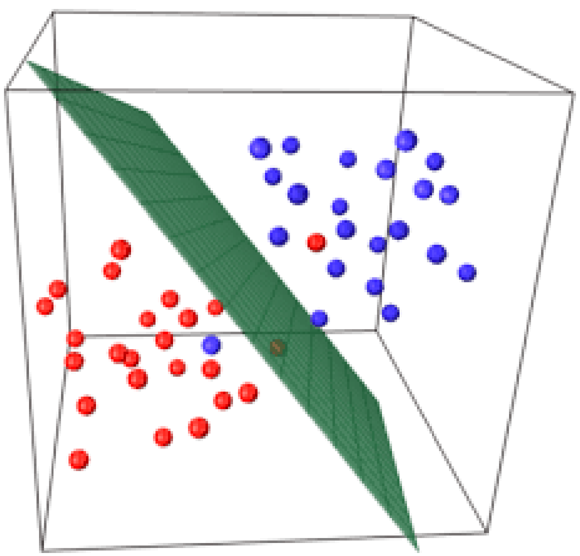
Photo: https://ww2.mathworks.cn/help/stats/create-and-visualize-discriminant-analysis-classifier.html

Classification problem

- Linear models for classification: the decision surfaces are linear functions of the input vector $\mathbf{x}$



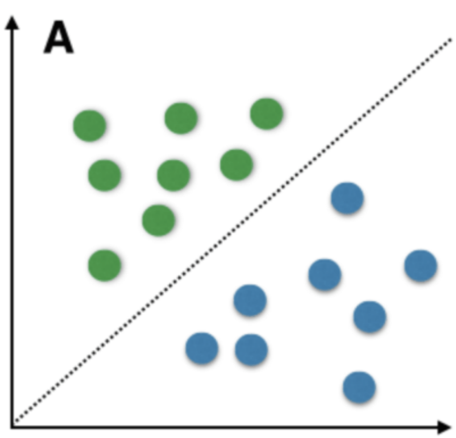
2D case



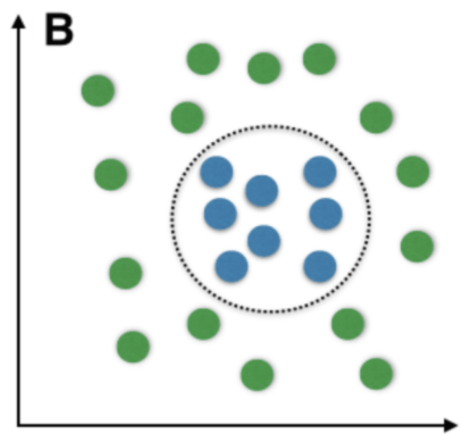
3D case

Classification problem

- Linear models for classification: the decision surfaces are linear functions of the input vector $\mathbf{x}$
- The decision surfaces are defined by $(D-1)$-dimensional hyperplanes within the D-dimensional input space
- Data whose classes can be separated by linear decision surfaces are said to be linearly separable



linearly separable



not linearly separable

Classification problem

- Given a training data set comprising N observations $\{\mathbf{x}_n\}_{n=1}^{N}$ and the corresponding target labels $\{t_n\}_{n=1}^{N}$, the goal of classification is to predict the label of t for a new data sample of $\mathbf{x}$
  - Categorical outputs, e.g., yes/no, dog/cat/other, called labels
  - A classifier assigns each input vector to one of these labels
- Binary classification: two possible labels
- Multi-class classification: multiple possible labels
- Label representation
  - Two classes: $t \in \{1,0\}$ or $t \in \{+1,-1\}$
  - Multiple classes, e.g., $K = 5$: $t = (0, 1, 0, 0, 0)^{\mathrm{T}}$ (1-of-*K* scheme)

Three representative linear classifiers

- Different linear models for classification
  - Discriminant functions
  - Generative approach using Bayes' theorem: $p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})}$
  - Discriminative approach to directly model the class-conditional density: $p(\mathcal{C}_k|\mathbf{x})$

Linear discriminant for two-class classification

- A linear discriminant is a linear function that takes an input vector $\mathbf{x}$ and assigns it to one of K classes
- A linear discriminant function for two-class classification

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

  where $\mathbf{w}$ is the weight vector and w_0 is the bias

- The decision boundary is $y(\mathbf{x}) = 0$, i.e., classification result

$$\begin{cases} C_1\,, & \text{if } y(\mathbf{x}) \geq 0\,, \\ C_2\,, & \text{otherwise}\,. \end{cases}$$

- $y(\mathbf{x}) = 0$ is a $(D-1)$-dimensional hyperplane within the D-dimensional input space

Properties of a linear discriminant

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

- Weight vector $\mathbf{w}$ is orthogonal to every vector lying within the decision boundary
  - Consider two points $\mathbf{x}_A$ and $\mathbf{x}_B$, which lie on the decision boundary
  - We have $y(\mathbf{x}_{\mathrm{A}}) = y(\mathbf{x}_{\mathrm{B}}) = 0$, leading to

$$\mathbf{w}^{\mathrm{T}}(\mathbf{x}_{\mathrm{A}} - \mathbf{x}_{\mathrm{B}}) = 0$$

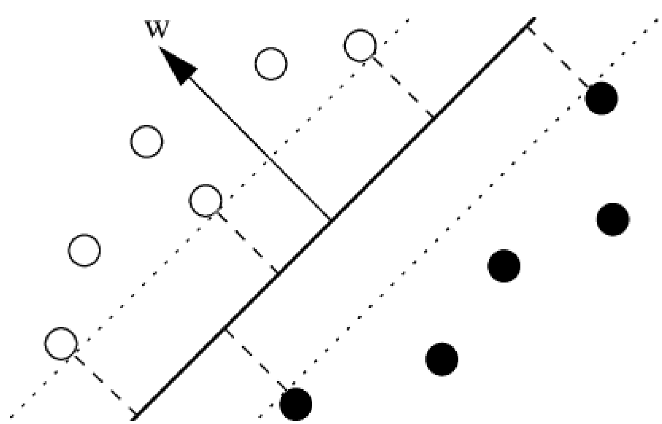


Photo: K.-R. Muller

Properties of a linear discriminant

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

- The distance from the origin to the decision boundary is

$$\frac{\mathbf{w}^{\mathrm{T}}\mathbf{x}}{\|\mathbf{w}\|} = -\frac{w_0}{\|\mathbf{w}\|}$$

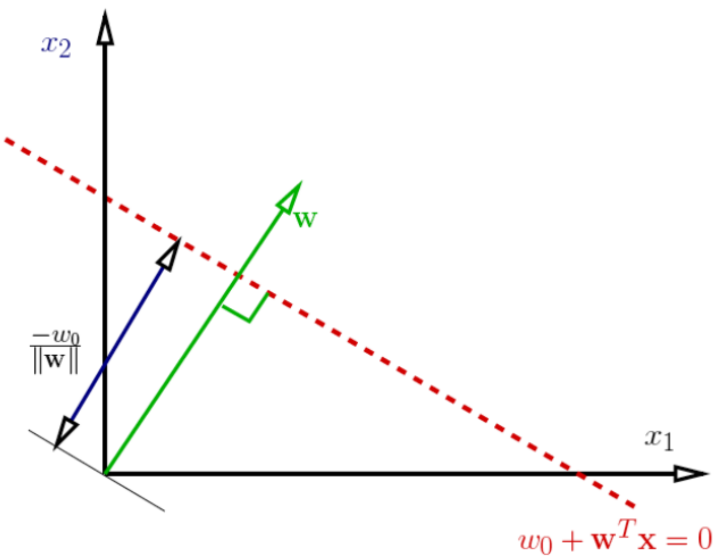
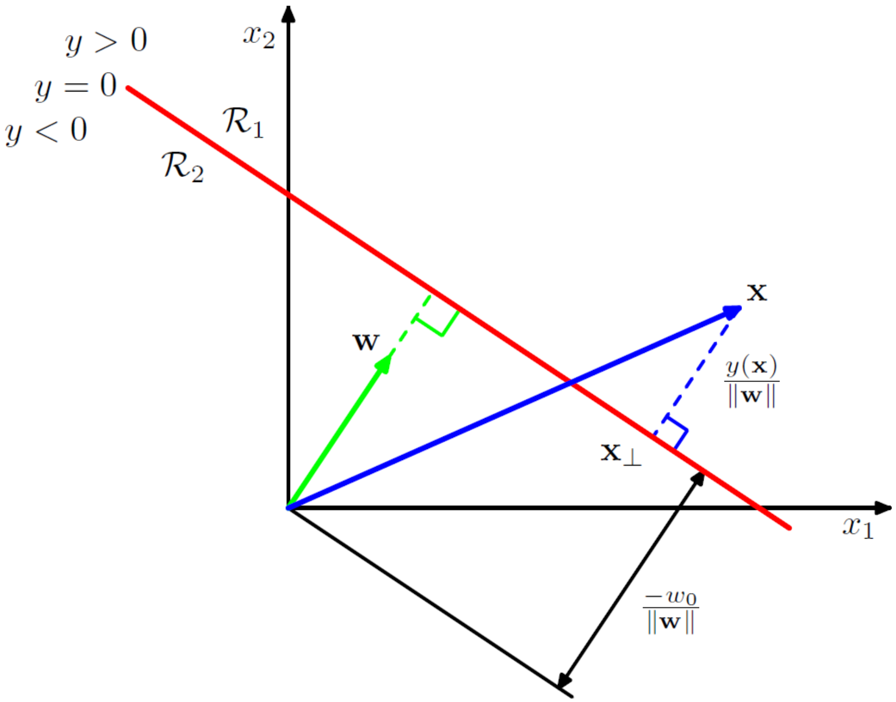


Photo: G. Shakhnarovich

Properties of a linear discriminant

- How to compute the distance between an arbitrary point $\mathbf{x}$ to the decision boundary $y(\mathbf{x}) = 0$?



$$\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

$$\begin{cases} y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0 \\ y(\mathbf{x}_\perp) = \mathbf{w}^{\mathrm{T}}\mathbf{x}_\perp + w_0 = 0 \end{cases}$$

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0 = \mathbf{w}^{\mathrm{T}}\mathbf{x}_\perp + w_0 + r\frac{\mathbf{w}^{\mathrm{T}}\mathbf{w}}{\|\mathbf{w}\|}$$

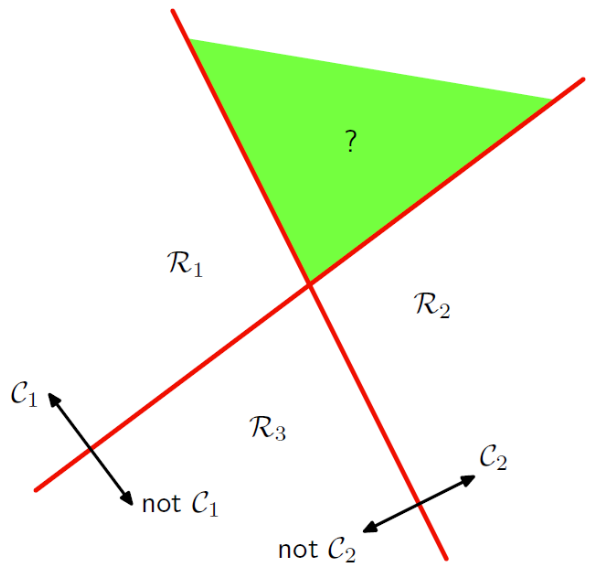
$$r = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}$$

Linear discriminant for multi-class classification

- Consider the extension of linear discriminants to $K > 2$ classes
- Many classifiers cannot directly extend to multi-class classification
  - Build a K-class discriminant by combining a number of two-class discriminant functions
  - One-versus-the-rest strategy
  - One-versus-one strategy

One-versus-the-rest

- One-vs-the-rest
  - Learn $K-1$ two-class classifiers (linear discriminants)
  - Classifier 1 is derived to separate data of class 1 from the rest
  - Classifier 2 is derived to separate data of class 2 from the rest
  - …
  - Classifier $K-1$ is derived to separate data of class $K-1$ from the rest



3-class classification

2 one-vs-the-rest linear discriminants

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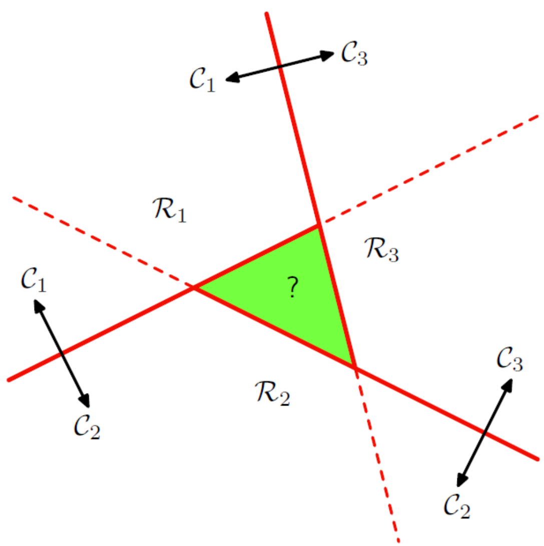
One-vs-one

- One-vs-one
  - Learn $K(K-1)/2$ two-class classifiers, one for each class pair
  - For classes *i* and *j*, a binary classifier is learned to separate data of class *i* from those of class *j*
  - Classification is done by majority vote
- The problem of ambiguous regions



3-class classification

3 one-vs-one linear discriminants

K-class discriminant

- A single *K*-class discriminant can avoid the problem of ambiguous regions
  - It is composed of *K* linear functions of the form

$$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$

for $k = 1, 2, \dots K$

  - It assigns a point $\mathbf{x}$ to class *k* if

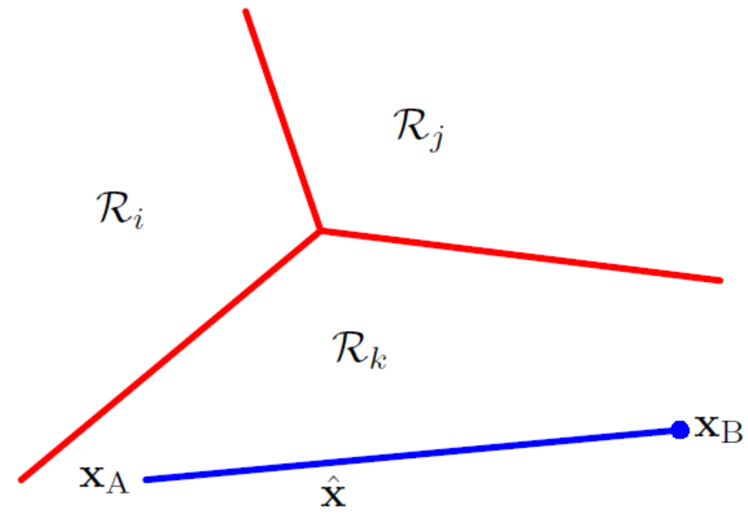
$$y_k(\mathbf{x}) > y_j(\mathbf{x}) \text{ for all } j \neq k$$

  - The decision boundary between class *k* and class *j* is

$$y_k(\mathbf{x}) = y_j(\mathbf{x})$$

$$\Rightarrow (\mathbf{w}_k - \mathbf{w}_j)^{\mathrm{T}}\mathbf{x} + (w_{k0} - w_{j0}) = 0$$

K-class discriminant



- An example: 3-class discriminant
- The decision regions of such a discriminant are convex
- Consider two points $\mathbf{x}_A$ and $\mathbf{x}_B$, which lie inside region $\mathcal{R}_k$
- For any point $\hat{\mathbf{x}}$ that lies on the line connecting $\mathbf{x}_A$ and $\mathbf{x}_B$, it can be expressed as

$$\widehat{\mathbf{x}} = \lambda \mathbf{x}_\mathrm{A} + (1 - \lambda)\mathbf{x}_\mathrm{B} \quad \text{where } 0 \leqslant \lambda \leqslant 1$$

- It can be proved that $\hat{\mathbf{x}}$ also lies inside $\mathcal{R}_k$
  - Linear function of class *k*: $y_k(\hat{\mathbf{x}}) = \lambda y_k(\mathbf{x}_A) + (1 - \lambda) y_k(\mathbf{x}_B)$
  - Proof: $y_k(\mathbf{x}_A) > y_j(\mathbf{x}_A), y_k(\mathbf{x}_B) > y_j(\mathbf{x}_B)$, for all $j \neq k$
    $\Rightarrow y_k(\hat{\mathbf{x}}) > y_j(\hat{\mathbf{x}})$

Linear discriminant learning

- Learning focuses on estimating a good decision boundary
- We need to optimize parameters $\boldsymbol{w}$ and w_0 of the boundary
- What does good mean here?
- Is this boundary good

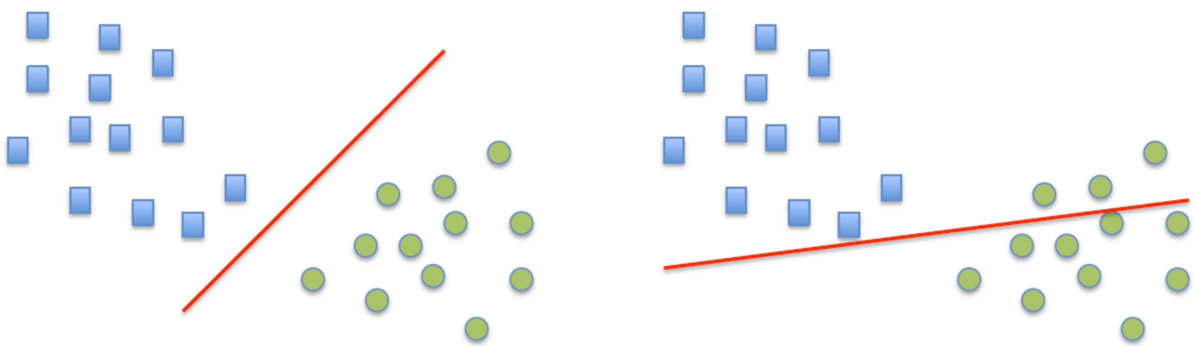


Photo: R. Zemel et al.

- We need a criterion to tell how to optimize these parameters

Least squares for classification

- Use least squares technique to solve a *K*-class discriminant
- Each class *k* is described by its own linear model

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

- A point $\mathbf{x}$ is assigned to class *k* if

$$y_k(\mathbf{x}) > y_j(\mathbf{x}) \text{ for all } j \neq k$$

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Least squares for classification

- Some notations
  - A data point $\mathbf{x}$: $\widetilde{\mathbf{x}} = (1, \mathbf{x}^{\mathrm{T}})^{\mathrm{T}}$
  - 1-of-*K* binary coding for the label vector of $\mathbf{x}$: $\mathbf{t} = [0,1,0,0,0]^T$
  - The linear model for class *k*: $\widetilde{\mathbf{w}}_k = (w_{k0}, \mathbf{w}_k^{\mathrm{T}})^{\mathrm{T}}$
  - Apply the linear model for class *k* to a point $\mathbf{x}$: $y_k = \widetilde{\mathbf{w}}_k^{\mathrm{T}} \widetilde{\mathbf{x}}$
  - All data points: $\widetilde{\mathbf{X}} = \begin{bmatrix} \widetilde{\mathbf{x}}_1^{\mathrm{T}} \\ \vdots \\ \widetilde{\mathbf{x}}_N^{\mathrm{T}} \end{bmatrix}$ All data label vectors: $\widetilde{\mathbf{T}} = \begin{bmatrix} \mathbf{t}_1^{\mathrm{T}} \\ \vdots \\ \mathbf{t}_N^{\mathrm{T}} \end{bmatrix}$
  - All linear models: $\widetilde{\mathbf{W}} = [\widetilde{\mathbf{w}}_1, \widetilde{\mathbf{w}}_2, \ldots, \widetilde{\mathbf{w}}_K]$
  - Apply all linear models to a point $\mathbf{x}$: $\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^{\mathrm{T}} \widetilde{\mathbf{x}}$

Least squares for classification

- The squared difference between $\mathbf{t}$ and $\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^{\mathrm{T}}\widetilde{\mathbf{x}}$
- Sum-of-squares error

$$E_D(\widetilde{\mathbf{W}}) = \frac{1}{2}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\}$$

- Proof sketch
  - Tr(*AB*) = Tr(*BA*)
  - Tr(*BA*) is the sum of the diagonal elements of square matrix *BA*
  - The *n*th diagonal element is the squared error of point $\mathbf{x}_n$
- Setting the derivative w.r.t. $\widetilde{\mathbf{W}}$ to 0, we obtain

$$\widetilde{\mathbf{W}} = (\widetilde{\mathbf{X}}^{\mathrm{T}}\widetilde{\mathbf{X}})^{-1}\widetilde{\mathbf{X}}^{\mathrm{T}}\mathbf{T} = \widetilde{\mathbf{X}}^{\dagger}\mathbf{T}$$

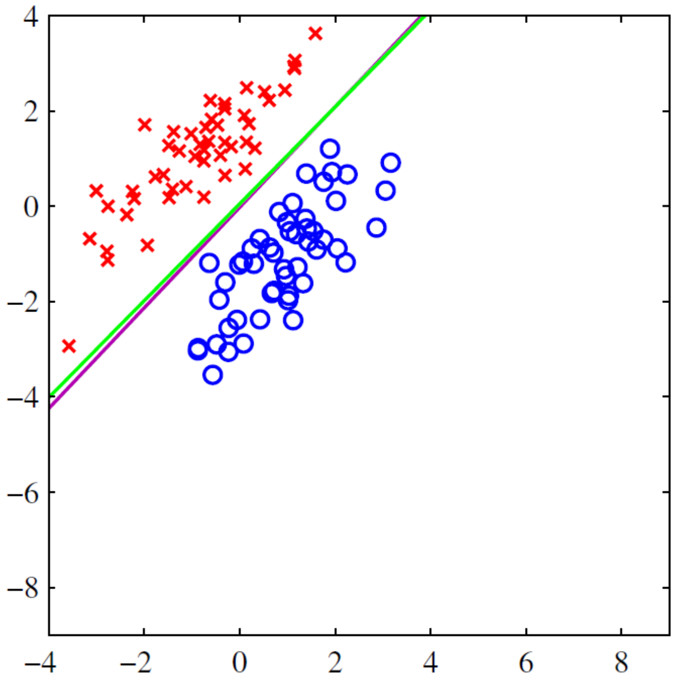
Least squares for classification

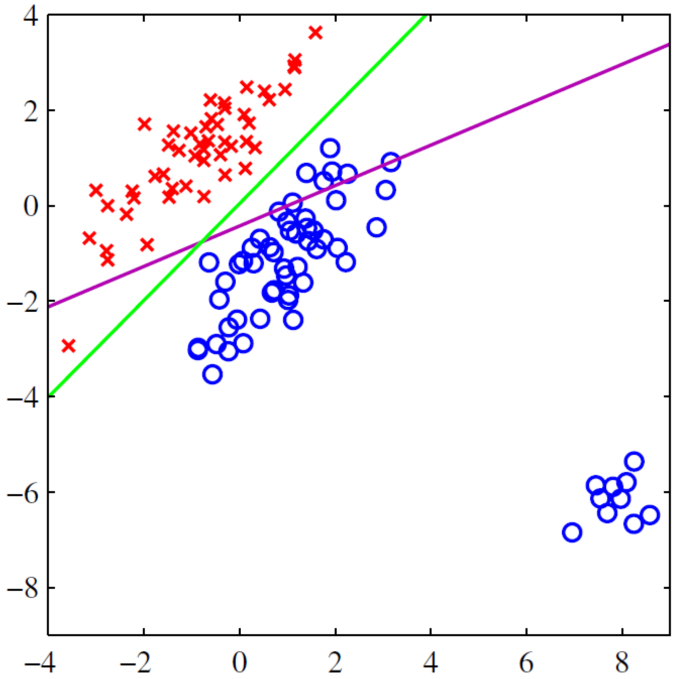
- After getting $\widetilde{\mathbf{W}}$, we classify a new data point via

$$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^{\mathrm{T}}\widetilde{\mathbf{x}} = \mathbf{T}^{\mathrm{T}}\left(\widetilde{\mathbf{X}}^{\dagger}\right)^{\mathrm{T}}\widetilde{\mathbf{x}}$$

Least squares for classification

- The least-squares solutions are sensitive to outliers





Magenta: least squares

Green: logistic regression

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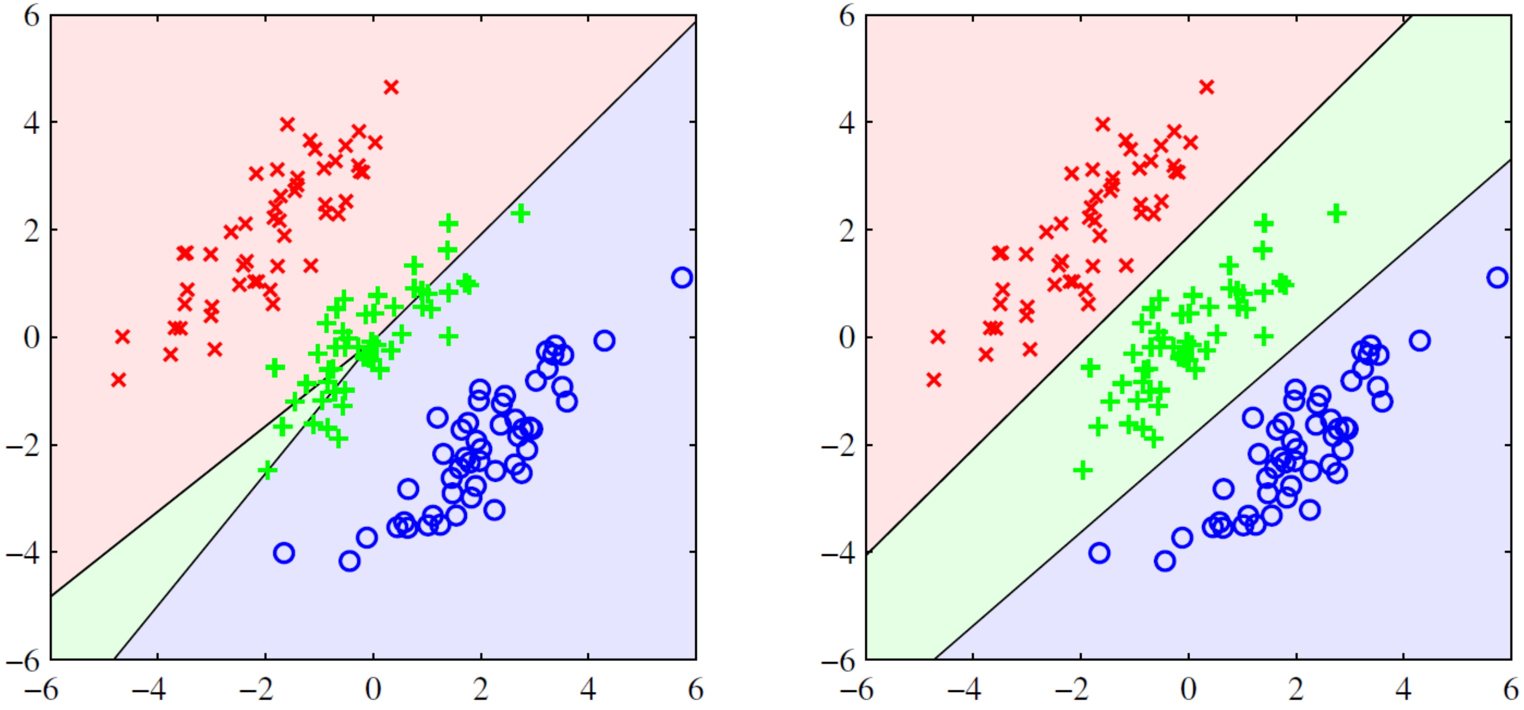
Least squares for classification

- The least squares method sometimes gives poor results



Left: least squares
Right: logistic regression

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Fisher's linear discriminant: 2 classes

- Fisher's linear discriminant (FLD): a non-probabilistic method for dimensionality reduction

- Consider the case of two classes, and suppose we take a D-dimensional input vector $\mathbf{x}$ and project it onto one dimension by

$$y = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

- If we place a threshold on $\mathbf{x}$, and classify it as class C_1 if $y \geq -w_0$, and otherwise class C_2, we get the linear classifier discussed previously

- In general, dimensionality reduction leads to information loss, but we can select a projection maximizing data separation

Linear discriminant with maximum separation

- A two-class problem where there are N_1 points of class C_1 and N_2 points of class C_2
- The mean vectors of the two classes are

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in \mathcal{C}_1} \mathbf{x}_n \quad \text{and} \quad \mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in \mathcal{C}_2} \mathbf{x}_n$$

- An intuitive choice of $\mathbf{w}$ that maximizes the distance between the projected mean vectors, i.e.,

$$m_2 - m_1 = \mathbf{w}^{\mathrm{T}}(\mathbf{m}_2 - \mathbf{m}_1)$$

$$\text{where} \quad m_k = \mathbf{w}^{\mathrm{T}}\mathbf{m}_k$$

- However, the distance can be arbitrarily large by increasing the magnitude of $\mathbf{w}$

Linear discriminant with maximum separation

- We constrain $\mathbf{w}$ to have unit length, i.e., $\sum_i w_i^2 = 1$
- The constrained optimization problem:

$$\text{Maximize } \mathbf{w}^{\mathrm{T}}(\mathbf{m}_2 - \mathbf{m}_1)\,,$$
$$\text{subject to } \mathbf{w}^{\mathrm{T}}\mathbf{w} = 1\,.$$

- The optimal $\mathbf{w}$ in the optimization problem above

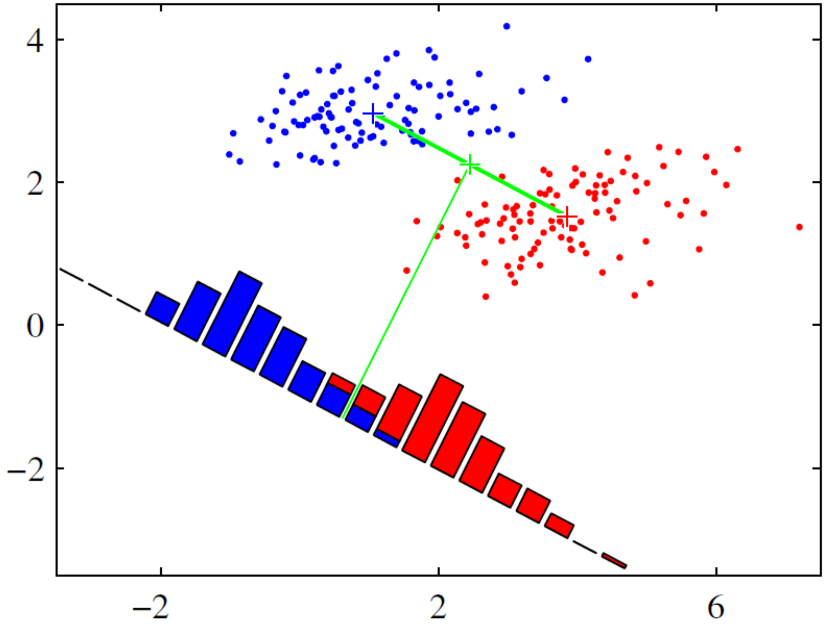
$$\mathbf{w} \propto (\mathbf{m}_2 - \mathbf{m}_1)$$

- How to prove?
  - Use Lagrange multiplier to solve it
  - By setting the gradient of Lagrange function w.r.t. optimization variables to 0, we get

$$(\mathbf{m}_2 - \mathbf{m}_1) + 2\lambda\mathbf{w} = 0$$

Linear discriminant with maximum separation

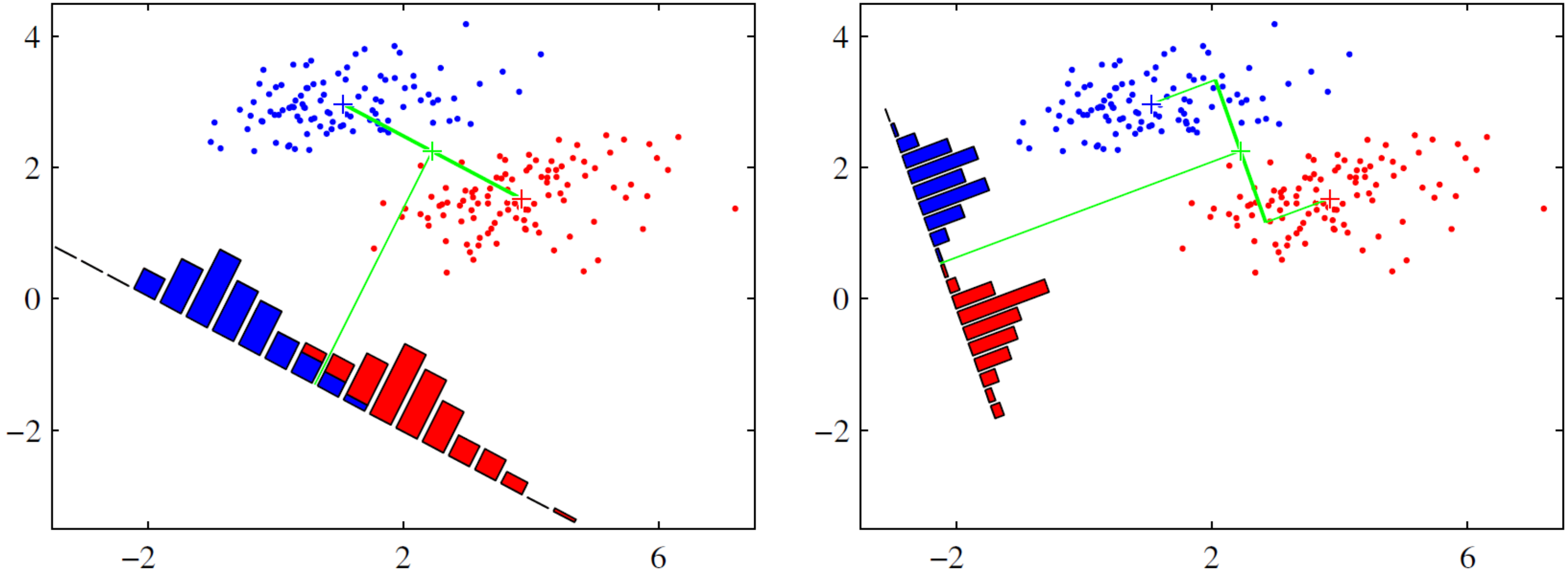
- Is the obtained $\mathbf{w} \propto (\mathbf{m}_2 - \mathbf{m}_1)$ good?



  - $+$: $\mathbf{m}_1$, $+$: $\mathbf{m}_2$, $+$: threshold
  - Histograms of the two classes overlap

Linear discriminant with maximum separation

- Is the obtained $\mathbf{w} \propto (\mathbf{m}_2 - \mathbf{m}_1)$ good?



- ➢ +: $\mathbf{m}_1$, +: $\mathbf{m}_2$, +: threshold
- ➢ Histograms of the two classes overlap
- ➢ Right plot: The projection learned by FLD

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Fisher's linear discriminant: 2 classes

- FLD seeks the projection $\mathbf{w}$ that gives a large distance between the projected data means while giving a small variance within each class

- Maximize the between-class variance

$$(m_2 - m_1)^2 \quad \text{where} \quad m_k = \mathbf{w}^{\mathrm{T}}\mathbf{m}_k$$

- Minimize the within-class variance

$$s_k^2 = \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2 \quad \text{where} \quad y_n = \mathbf{w}^{\mathrm{T}}\mathbf{x}_n$$

- The objective (Fisher criterion):

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

Fisher's linear discriminant: 2 classes

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

- The objective (Fisher criterion):

$$J(\mathbf{w}) = \frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w}}$$

where S_{B} is the between-class covariance matrix

$$\mathbf{S}_{\mathrm{B}} = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^{\mathrm{T}}$$

S_{W} is the within-class covariance matrix

$$\mathbf{S}_{\mathrm{W}} = \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^{\mathrm{T}} + \sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^{\mathrm{T}}$$

Fisher's linear discriminant: 2 classes

$$J(\mathbf{w}) = \frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w}}$$

- Differentiate Fisher criterion w.r.t. $\mathbf{w}$

$$\frac{\partial}{\partial \mathbf{w}} J(\mathbf{w}) = 0$$

$$\frac{2\mathbf{S}_{\mathrm{B}}\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w}} + \frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}}{(\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w})^2}(-2\mathbf{S}_{\mathrm{W}}\mathbf{w}) = 0$$

- We find that

$$\underbrace{(\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w})}_{\text{scalar}}\mathbf{S}_{\mathrm{W}}\mathbf{w} = \underbrace{(\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w})}_{\text{scalar}}\mathbf{S}_{\mathrm{B}}\mathbf{w}$$

- As $\mathbf{S}_{\mathrm{B}}\mathbf{w} = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^{\mathrm{T}}\mathbf{w}$, $\mathbf{S}_{\mathrm{B}}\mathbf{w}$ is in the direction of $(\mathbf{m}_2 - \mathbf{m}_1)$
- We have

$$\mathbf{w} \propto \mathbf{S}_{\mathrm{W}}^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

Fisher's linear discriminant: 2 classes

- The optimized $\mathbf{w}$ is called Fisher's linear discriminant
- Project training data into a one-dimensional space via $\mathbf{w}$
  - Classification can be carried out by several methods
  - Determine a threshold y_0
    - Predict a point $\mathbf{x}$ as C_1 if $y(\mathbf{x}) \geq -y_0$, and otherwise class C_2
  - Use the nearest-neighbor rule
    - Project all training data into the one-dimensional space via $\mathbf{w}$
    - Project a testing point $\mathbf{x}$ to the same space
    - Retrieve the nearest training sample of $\mathbf{x}$ in the projected space
    - Predict $\mathbf{x}$ as the class that the retrieved sample belongs to

Fisher's linear discriminant: Multiple classes

- Fisher's linear discriminant (FLD) for $K > 2$ classes
- Assume the dimension of the input space is D, which is greater than K
- FLD introduces $D' \geq 1$ linear weight vectors $y_k = \mathbf{w}_k^{\mathrm{T}}\mathbf{x}$ for $k = 1, \ldots, D'$
- Gathering the weight vectors together projects each data point $\mathbf{x}$ to a D'-dimensional space

$$\mathbf{y} = \mathbf{W}^{\mathrm{T}}\mathbf{x}$$

where weight vectors $\{\mathbf{w}_k\}$ are the columns of $\mathbf{W}$

Fisher's linear discriminant: Multiple classes

- Generalize the within-class covariance matrix to K classes
- Recall the within-class covariance matrix when $K = 2$

$$\mathbf{S}_{\mathrm{W}} = \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^{\mathrm{T}} + \sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^{\mathrm{T}}$$

- The within-class covariance matrix when $K \geq 2$

$$\mathbf{S}_{\mathrm{W}} = \sum_{k=1}^{K} \mathbf{S}_k$$

where

$$\mathbf{S}_k = \sum_{n \in \mathcal{C}_k} (\mathbf{x}_n - \mathbf{m}_k)(\mathbf{x}_n - \mathbf{m}_k)^{\mathrm{T}} \quad \text{and} \quad \mathbf{m}_k = \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} \mathbf{x}_n$$

Fisher's linear discriminant: Multiple classes

- Recall the between-class covariance matrix when $K = 2$

$$\mathbf{S}_{\mathrm{B}} = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^{\mathrm{T}}$$

- The extended between-class covariance matrix for $K > 2$

$$\mathbf{S}_{\mathrm{B}} = \sum_{k=1}^{K} N_k(\mathbf{m}_k - \mathbf{m})(\mathbf{m}_k - \mathbf{m})^{\mathrm{T}}$$

where

$$\mathbf{m} = \frac{1}{N}\sum_{n=1}^{N} \mathbf{x}_n$$

Fisher's linear discriminant: Multiple classes

- Consider the case where FLD projects data to a one-dimensional space, i.e., $D' = 1$

$$J(\mathbf{w}) = \frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w}}$$

- An equivalent objective

$$\begin{aligned} \min_{\mathbf{w}} \quad & -\frac{1}{2}\mathbf{w}^T S_B \mathbf{w} \\ \text{s.t.} \quad & \mathbf{w}^T S_W \mathbf{w} = 1 \end{aligned}$$

- Lagrangian function

$$\mathcal{L}_P = -\frac{1}{2}\mathbf{w}^T S_B \mathbf{w} + \frac{1}{2}\lambda(\mathbf{w}^T S_W \mathbf{w} - 1)$$

- We have $S_B \mathbf{w} = \lambda S_W \mathbf{w} \quad \Rightarrow \quad S_W^{-1} S_B \mathbf{w} = \lambda \mathbf{w}$
- The optimal **w** is the eigenvector of $S_W^{-1} S_B$ that corresponds to the largest eigenvalue

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Fisher's linear discriminant: Multiple classes

- Consider the case where FLD projects data to a multi-dimensional space, i.e., $D' > 1$
- Can we directly extend the objective to learn a multi-dimensional projection? No

$$J(\mathbf{w}) = \frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w}} \quad \Longrightarrow \quad J(\mathrm{w}) = \frac{\mathrm{W}^{\mathrm{T}}\mathrm{S}_{\mathrm{B}}\mathrm{W}}{\mathrm{W}^{\mathrm{T}}\mathrm{S}_{\mathrm{W}}\mathrm{W}}$$

- A choice for the objective is

$$J(\mathbf{w}) = \mathrm{Tr}\left\{(\mathbf{W}\mathbf{S}_{\mathrm{W}}\mathbf{W}^{\mathrm{T}})^{-1}(\mathbf{W}\mathbf{S}_{\mathrm{B}}\mathbf{W}^{\mathrm{T}})\right\}$$

- The columns of the optimal W are the eigenvectors of $S_W^{-1}S_B$ that correspond to the D' largest eigenvalues

Fisher's linear discriminant: Multiple classes

- About the value D', the dimension of the projected space

- Note that the rank of the between-class covariance matrix is at most $K - 1$

$$\mathbf{S}_{\mathrm{B}} = \sum_{k=1}^{K} N_k (\mathbf{m}_k - \mathbf{m})(\mathbf{m}_k - \mathbf{m})^{\mathrm{T}}$$

- In other words, the dimension of the projected space by FLD is at most $K - 1$

Probabilistic generative models: Two-class case

- In a generative model, we model the class-conditional densities $p(\mathbf{x}|\mathcal{C}_k)$ and class priors $p(\mathcal{C}_k)$, and then use them to compute posterior probabilities $p(\mathcal{C}_k|\mathbf{x})$ via Bayes' theorem
- Consider two-class cases. The posterior probability for class C_1 is defined by

$$\begin{aligned} p(\mathcal{C}_1|\mathbf{x}) &= \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \\ &= \frac{1}{1+\exp(-a)} = \sigma(a) \end{aligned}$$

where $\sigma(a)$ is the logistic sigmoid function

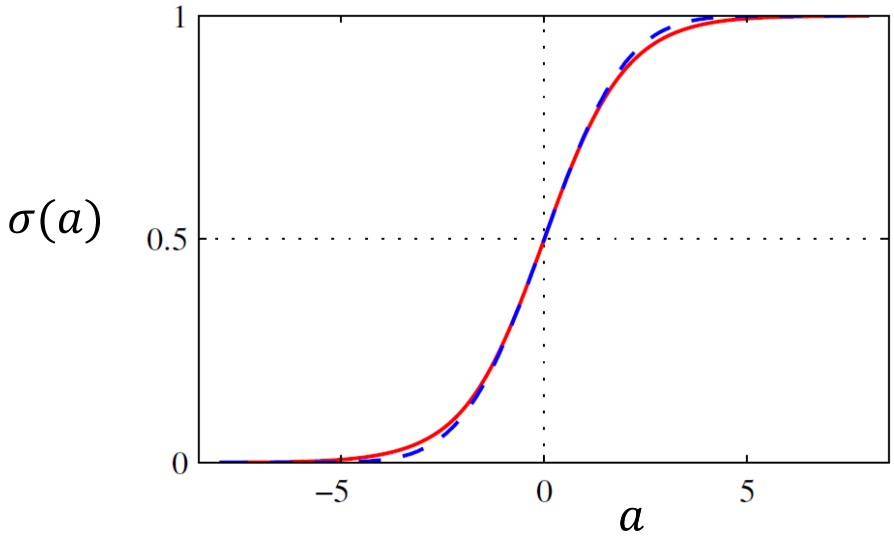
$$\sigma(a) = \frac{1}{1+\exp(-a)} \qquad a = \ln \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

Logistic sigmoid function

- Logistic sigmoid function maps the whole real axis into [0,1]
  - Symmetric property: $\sigma(-a) = 1 - \sigma(a)$
- The variable a here represents the log of the ratio of probabilities

$$\ln\left[p(\mathcal{C}_1|\mathbf{x})/p(\mathcal{C}_2|\mathbf{x})\right]$$

- Logistic sigmoid function (red curve)



Probabilistic generative models: Multi-class case

- For the case of $K > 2$ classes, the posterior probability for class C_k is defined by

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

where $a_k = \ln p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$

- Multi-class generalization of logistic sigmoid function, or softmax function
  - If $a_k \gg a_j$ for all $j \neq k$, we have $p(\mathcal{C}_k|\mathbf{x}) \simeq 1$ and $p(\mathcal{C}_j|\mathbf{x}) \simeq 0$

Continuous inputs: Two-class case

- Assume that the class-conditional densities are Gaussian and all classes share the same covariance matrix:

$$p(\mathbf{x}|\mathcal{C}_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\mathbf{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^{\mathrm{T}}\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k)\right\}$$

- Recall $p(\mathcal{C}_1|\mathbf{x}) = \sigma(a)$ where $a = \ln \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$

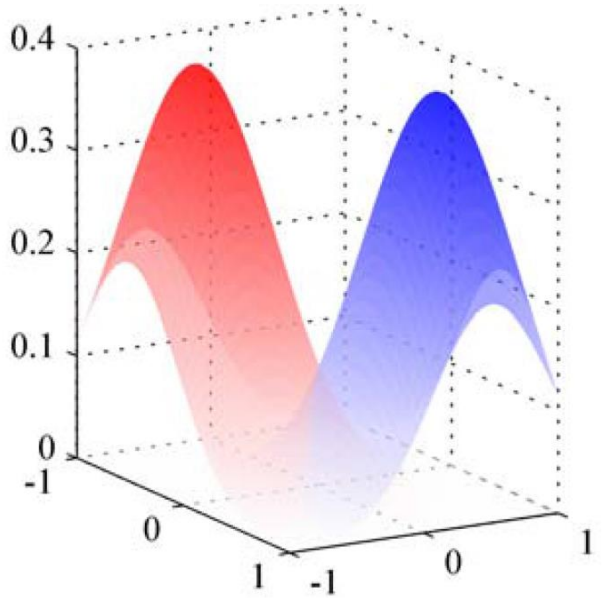
- We have $p(\mathcal{C}_1|\mathbf{x}) = \sigma(\mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0)$

where

$$\begin{aligned} \mathbf{w} &= \mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \\ w_0 &= -\frac{1}{2}\boldsymbol{\mu}_1^{\mathrm{T}}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^{\mathrm{T}}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 + \ln\frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)} \end{aligned}$$

- Note that the quadratic terms in $\mathbf{x}$ are canceled

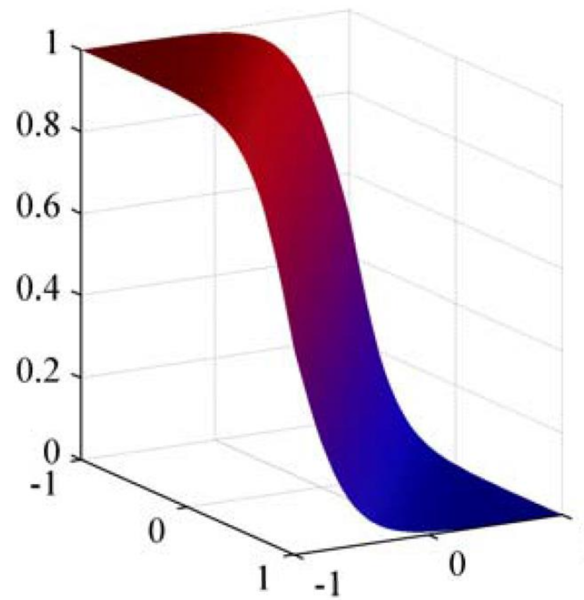
Class-conditional and posterior probabilities



class-conditional densities

$p(\mathbf{x}|\mathcal{C}_1)$: red

$p(\mathbf{x}|\mathcal{C}_2)$: blue



posterior probability

$p(\mathcal{C}_1|\mathbf{x})$

Note that $p(\mathcal{C}_2|\mathbf{x}) = 1 - p(\mathcal{C}_1|\mathbf{x})$

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Continuous inputs: Multi-class case

- Assume that the class-conditional densities are Gaussian and all classes share the same covariance matrix:

$$p(\mathbf{x}|\mathcal{C}_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k)\right\}$$

- Recall $p(\mathcal{C}_k|\mathbf{x}) = \dfrac{\exp(a_k)}{\sum_j \exp(a_j)}$ where $a_k = \ln p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$

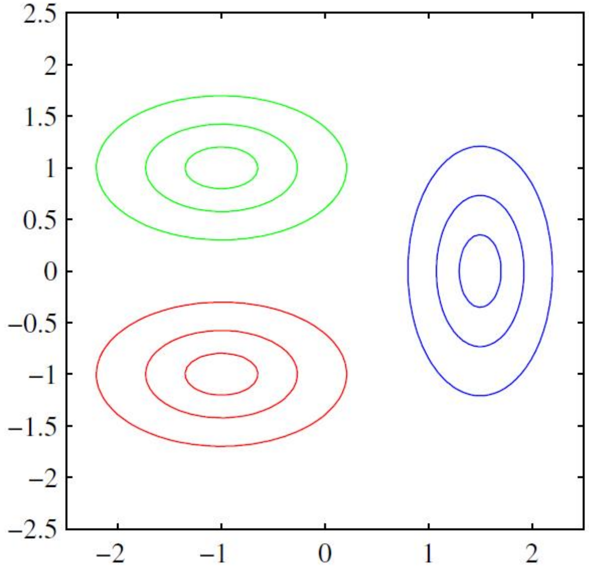
- We have $a_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$

where

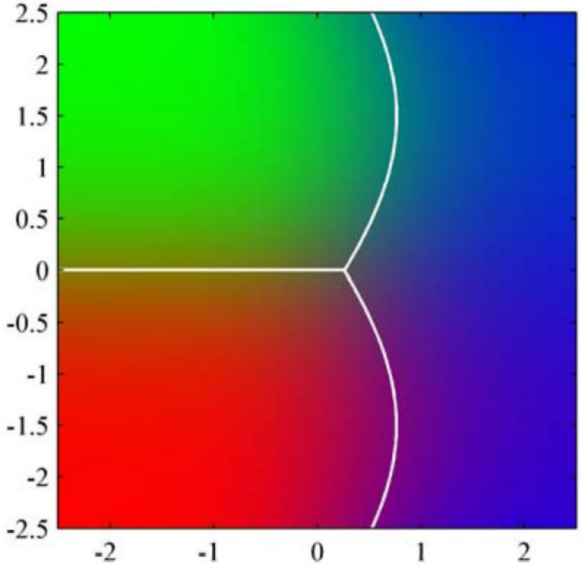
$$\begin{aligned} \mathbf{w}_k &= \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k \\ w_{k0} &= -\frac{1}{2}\boldsymbol{\mu}_k^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \ln p(\mathcal{C}_k) \end{aligned}$$

Continuous inputs: Multi-class case

- If each class-conditional density $p(\mathbf{x}|\mathcal{C}_k)$ has its own covariance matrix $\mathbf{\Sigma}_k$, it leads to a quadratic discriminant



three class-conditional densities



posterior probability

Decision boundary between red and green classes is linear, while those between other pairs are quadratic

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Determine parameter values via maximum likelihood

- We specify the functional form of class-conditional density

$$p(\mathbf{x}|\mathcal{C}_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\mathbf{\Sigma}|^{1/2}} \exp\left\{ -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^{\mathrm{T}} \mathbf{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu}_k) \right\}$$

- We assume the prior class probability takes the form

$$p(\mathcal{C}_1) = \pi \quad \text{and} \quad p(\mathcal{C}_2) = 1 - \pi$$

- Suppose a set of N data points $\{\mathbf{x}_n, t_n\}$ is provided, where $t_n = 1$ denotes class C_1 and $t_n = 0$ denotes class C_2

- Our goal is to determine the values of parameters $\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \mathbf{\Sigma}$ to complete classification

Determine parameter values via maximum likelihood

- For a data point $\mathbf{x}_n$ from class C_1, we have

$$p(\mathbf{x}_n, \mathcal{C}_1) = p(\mathcal{C}_1)p(\mathbf{x}_n|\mathcal{C}_1) = \pi\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \boldsymbol{\Sigma})$$

- Similarly for class C_2, we have

$$p(\mathbf{x}_n, \mathcal{C}_2) = p(\mathcal{C}_2)p(\mathbf{x}_n|\mathcal{C}_2) = (1-\pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

- Suppose data are i.i.d. The likelihood function is given by

$$p(\mathbf{t}|\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} [\pi\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \boldsymbol{\Sigma})]^{t_n} [(1-\pi)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_2, \boldsymbol{\Sigma})]^{1-t_n}$$

where $\mathbf{t} = (t_1, \ldots, t_N)^{\mathrm{T}}$

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Maximum likelihood solution for π

- It is convenient to maximize the log of the likelihood function
- Consider first the maximization w.r.t. π
- The terms in the log likelihood function that depend on π are

$$\sum_{n=1}^{N} \{t_n \ln \pi + (1 - t_n) \ln(1 - \pi)\}$$

- Setting the derivative w.r.t. π to zero, we obtain

$$\pi = \frac{1}{N} \sum_{n=1}^{N} t_n = \frac{N_1}{N} = \frac{N_1}{N_1 + N_2}$$

where N_1 is the number of data in class C_1 and N_2 is the number of data in class C_2

- The ML estimate for π is simple the fraction of points in class C_1

Maximum likelihood solution for $\boldsymbol{\mu}_1$

- Consider the maximization w.r.t. $\boldsymbol{\mu}_1$
- We pick those terms that depend on $\boldsymbol{\mu}_1$ in the log likelihood function

$$\sum_{n=1}^{N} t_n \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}) = -\frac{1}{2}\sum_{n=1}^{N} t_n(\mathbf{x}_n - \boldsymbol{\mu}_1)^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_1) + \text{const}$$

- Setting the derivative w.r.t. $\boldsymbol{\mu}_1$ to zero leads to

$$\boldsymbol{\mu}_1 = \frac{1}{N_1}\sum_{n=1}^{N} t_n \mathbf{x}_n$$

- It is simply the mean of all data points belonging to class C_1

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Maximum likelihood solution for $\boldsymbol{\mu}_2$

- Similarly, the corresponding result for $\boldsymbol{\mu}_2$ is

$$\boldsymbol{\mu}_2 = \frac{1}{N_2} \sum_{n=1}^{N} (1 - t_n) \mathbf{x}_n$$

- It is simply the mean of all data points belonging to class C_2

Maximum likelihood solution for $\boldsymbol{\Sigma}$

- Finally, consider the maximum likelihood solution for the shared covariance matrix $\boldsymbol{\Sigma}$
- Picking out the terms in the log likelihood function that depend on $\boldsymbol{\Sigma}$, we get

$$
-\frac{1}{2}\sum_{n=1}^{N} t_n \ln|\boldsymbol{\Sigma}| - \frac{1}{2}\sum_{n=1}^{N} t_n (\mathbf{x}_n - \boldsymbol{\mu}_1)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_1)
$$

$$
-\frac{1}{2}\sum_{n=1}^{N} (1 - t_n) \ln|\boldsymbol{\Sigma}| - \frac{1}{2}\sum_{n=1}^{N} (1 - t_n)(\mathbf{x}_n - \boldsymbol{\mu}_2)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_2)
$$

$$
= -\frac{N}{2} \ln|\boldsymbol{\Sigma}| - \frac{N}{2} \mathrm{Tr}\left\{\boldsymbol{\Sigma}^{-1}\mathbf{S}\right\}
$$

Maximum likelihood solution for $\boldsymbol{\Sigma}$

where
$$\begin{aligned}
\mathbf{S} &= \frac{N_1}{N}\mathbf{S}_1 + \frac{N_2}{N}\mathbf{S}_2 \\
\mathbf{S}_1 &= \frac{1}{N_1}\sum_{n\in\mathcal{C}_1}(\mathbf{x}_n - \boldsymbol{\mu}_1)(\mathbf{x}_n - \boldsymbol{\mu}_1)^{\mathrm{T}} \\
\mathbf{S}_2 &= \frac{1}{N_2}\sum_{n\in\mathcal{C}_2}(\mathbf{x}_n - \boldsymbol{\mu}_2)(\mathbf{x}_n - \boldsymbol{\mu}_2)^{\mathrm{T}}.
\end{aligned}$$

- Setting the derivative to zero, we have $\boldsymbol{\Sigma} = \mathbf{S}$
- The derivation

$$\left.\begin{array}{l}
\frac{\partial}{\partial\boldsymbol{\Sigma}}\ln|\boldsymbol{\Sigma}| = (\boldsymbol{\Sigma}^{-1})^{\mathrm{T}} \\
\frac{\partial}{\partial\boldsymbol{\Sigma}}\mathrm{Tr}\boldsymbol{\Sigma}^{-1}\mathbf{S} = -(\boldsymbol{\Sigma}^{-1})^{\mathrm{T}}\mathbf{S}^{\mathrm{T}}(\boldsymbol{\Sigma}^{-1})^{\mathrm{T}}
\end{array}\right\} \Rightarrow (\boldsymbol{\Sigma}^{-1})^{\mathrm{T}} = (\boldsymbol{\Sigma}^{-1})^{\mathrm{T}}\mathbf{S}^{\mathrm{T}}(\boldsymbol{\Sigma}^{-1})^{\mathrm{T}}$$

Generative approach summary

- Class-conditional densities

$$p(\mathbf{x}|\mathcal{C}_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\mathbf{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^{\mathrm{T}}\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k)\right\}$$

- Class prior probabilities

$$p(\mathcal{C}_1) = \pi \quad \text{and} \quad p(\mathcal{C}_2) = 1 - \pi$$

- Determine the parameter values of $\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \mathbf{\Sigma}$
- Classification is carried out via

$$p(\mathcal{C}_1|\mathbf{x}) = \sigma(a) \quad \text{where} \quad a = \ln \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

$$p(\mathcal{C}_2|\mathbf{x}) = 1 - p(\mathcal{C}_1|\mathbf{x})$$

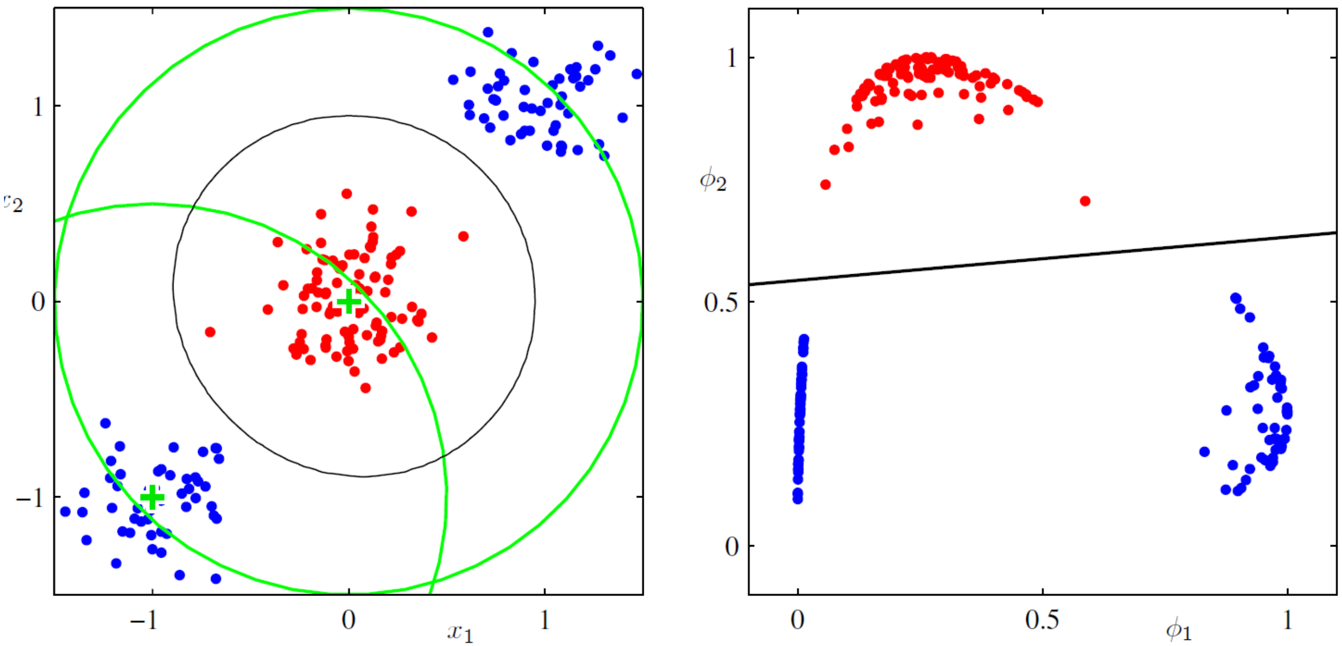
- ML solution can be directly extended to multi-class cases

Generative vs. Discriminative models

- Probabilistic generative model: Indirect approach that finds the parameters of class-conditional densities and class priors, and applies Bayes' theorem to get posterior probabilities
- Probabilistic discriminative models: Direct approach that uses the generalized linear model to represent posterior probabilities, and determines its parameters directly.
- Advantages of discriminative models:
  - Better performance in most cases, especially when the class-conditional density assumption gives a poor approximation to the true distribution
  - Less parameters

Nonlinear basis functions for linear classification

- Nonlinear basis functions help when dealing with data that are not linearly separable: $\mathbf{x} \to \phi(\mathbf{x})$



data points of class C_1

data points of class C_2

+: mean of Gaussian basis function

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Logistic regression for two-class classification

- Recall the posterior probability for two-class classification

$$\begin{aligned} p(\mathcal{C}_1|\mathbf{x}) &= \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)+p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \\ &= \frac{1}{1+\exp(-a)} = \sigma(a) \end{aligned}$$

- 1. Ignore the class-conditional probabilities and class priors
- 2. Apply basis functions for nonlinear transform
- 3. Assume the posterior probability can be written as a logistic sigmoid acting on a linear function of the feature vector
- We get

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma\left(\mathbf{w}^{\mathrm{T}}\phi\right) \quad \text{and} \quad p(\mathcal{C}_2|\phi) = 1 - p(\mathcal{C}_1|\phi)$$

where $\sigma(a) = \dfrac{1}{1+\exp(-a)}$

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Logistic regression model

- This model is called logistic regression, though it is used for classification

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma\left(\mathbf{w}^{\mathrm{T}}\phi\right)$$

- Suppose the dimension of ϕ is M. There are M parameters to learn in logistic regression

- Cf. For the generative model, we use $2M$ parameters for the means of two classes and $M\ (M+1)/2$ parameters for the shared covariance matrix

Determine parameters of logistic regression

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma\left(\mathbf{w}^{\mathrm{T}}\phi\right)$$

- The derivative of the logistic sigmoid function

$$\frac{d\sigma}{da} = \sigma(1-\sigma)$$

- Derivation:

$$\sigma(a) = \frac{1}{1+e^{-a}}$$
$$\frac{\partial\sigma}{\partial a} = \frac{1}{(1+e^{-a})^2}\cdot\left(e^{-a}\right) = \frac{1}{1+e^{-a}}\cdot\frac{e^{-a}}{1+e^{-a}} = \sigma(1-\sigma)$$

- Given training data $\{\phi_n, t_n\}$, where $t_n \in \{0,1\}$, $\phi_n = \phi(\mathbf{x}_n)$ for $n = 1,\ldots,N$, the likelihood function of logistic regression is

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n}\left\{1-y_n\right\}^{1-t_n}$$

where $\mathbf{t} = (t_1,\ldots,t_N)^{\mathrm{T}}$ and $y_n = p(\mathcal{C}_1|\phi_n)$

Determine parameters of logistic regression

- The negative log likelihood, called cross entropy error, is

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

where $y_n = \sigma(a_n)$ and $a_n = \mathbf{w}^{\mathrm{T}}\phi_n$

- The gradient of the error function w.r.t. $\mathbf{w}$ is

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

- Derivation:

Using $\frac{\partial\sigma}{\partial a} = (1-\sigma)\sigma$

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} \left\{ \frac{t_n}{y_n}(y_n(1-y_n))\phi_n - \frac{1-t_n}{1-y_n}(1-y_n)y_n\phi_n \right\}$$

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

Determine parameters of logistic regression

- Optimize the parameters by stochastic gradient descent

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n$$

- Optimize the parameters by iterative reweighted least squares (IRLS), i.e., Newton-Raphson iterative optimization scheme

$$\mathbf{w}^{(\text{new})} = \mathbf{w}^{(\text{old})} - \mathbf{H}^{-1} \nabla E(\mathbf{w})$$

where $\mathbf{H}$ is the Hessian matrix whose elements comprise the second derivatives of $E(\mathbf{w})$ w.r.t. $\mathbf{w}$

Newton-Raphson iterative optimization

- Negative log likelihood function

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

- Gradient

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n)\boldsymbol{\phi}_n = \boldsymbol{\Phi}^{\mathrm{T}}(\mathbf{y} - \mathbf{t})$$

- Hessian

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{n=1}^{N} y_n(1 - y_n)\boldsymbol{\phi}_n\boldsymbol{\phi}_n^{\mathrm{T}} = \boldsymbol{\Phi}^{\mathrm{T}}\mathbf{R}\boldsymbol{\Phi}$$

where $\mathbf{R}$ is a diagonal matrix with

$$R_{nn} = y_n(1 - y_n)$$

Newton-Raphson iterative optimization

- The Newton-Raphson update formula

$$\mathbf{w}^{(\text{new})} = \mathbf{w}^{(\text{old})} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$
$$= \mathbf{w}^{(\text{old})} - (\boldsymbol{\Phi}^{\mathrm{T}}\mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^{\mathrm{T}}(\mathbf{y} - \mathbf{t})$$

- Hessian matrix is positive definite
- Proof:

$\mathbf{R}$: $N \times N$ diagonal
$\mathbf{R}_{nn} = y_n(1 - y_n)$

$0 < y_n < 1$
$\Rightarrow \mathbf{v}^{\mathrm{T}}\mathbf{H}\mathbf{v} > 0$ for an arbitrary $\mathbf{v}$
$\Rightarrow \mathbf{H}$ is positive definite

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Multiclass logistic regression

- Recall two-class logistic regression

$$p(\mathcal{C}_1|\phi) = \sigma(a) = \sigma\left(\mathbf{w}^{\mathrm{T}}\phi\right) \quad \text{and} \quad p(\mathcal{C}_2|\phi) = 1 - p(\mathcal{C}_1|\phi)$$

where $\sigma(a) = \dfrac{1}{1 + \exp(-a)}$

- We deal with multiclass cases

$$p(\mathcal{C}_k|\phi) = y_k(\phi) = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

where the activation a_k is given by

$$a_k = \mathbf{w}_k^{\mathrm{T}}\phi$$

Likelihood function of multiclass logistic regression

- Two-class case: Given training data $\{\phi_n, t_n\}$, where $t_n \in \{0,1\}$, $\phi_n = \phi(\mathbf{x}_n)$ for $1,\ldots,N$, the likelihood function of two-class logistic regression is

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n}\{1-y_n\}^{1-t_n}$$

where $\mathbf{t} = (t_1,\ldots,t_N)^{\mathrm{T}}$ and $y_n = p(\mathcal{C}_1|\phi_n)$

- For a multiclass case, we use 1-of-K coding $(0\,0\,\cdots\,1\,\cdots\,0)^{\mathrm{T}}$ to represent each target label vector $\mathbf{t}_n$, let $y_{nk} = y_k(\phi_n)$, we have the likelihood function

$$p(\underbrace{\mathbf{T}}_{N\times K}|\mathbf{w}_1,\ldots,\mathbf{w}_K) = \prod_{n=1}^{N}\prod_{k=1}^{K} p(C_k|\phi_n)^{t_{nk}} = \prod_{n=1}^{N}\prod_{k=1}^{K} y_{nk}^{t_{nk}}$$

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Newton-Raphson iterative optimization

- Negative log likelihood function is

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

- When using Newton-Raphson iterative optimization, we need to have the following gradient and Hessian

$$\nabla_{\mathbf{w}_j} E(\mathbf{w}_1, \ldots, \mathbf{w}_K)$$

$$\nabla_{\mathbf{w}_k} \nabla_{\mathbf{w}_j} E(\mathbf{w}_1, \ldots, \mathbf{w}_K)$$

Background

- Variable dependence: $\mathbf{w} \rightarrow a \rightarrow y \rightarrow E$
- According to

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

we have

$$\frac{\partial E}{\partial y_{nk}} = -\frac{t_{nk}}{y_{nk}}$$

Background

- According to

$$p(\mathcal{C}_k|\phi) = y_k(\phi) = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

  we have

$$\frac{\partial y_k}{\partial a_j} = y_k(I_{kj} - y_j) \quad \text{where} \quad I_{kj} = \begin{cases} 1, & j = k, \\ 0, & \text{otherwise.} \end{cases}$$

- Proof

$$\frac{\partial y_k}{\partial a_k} = \frac{e^{a_k}}{\sum_i e^{a_i}} - \left(\frac{e^{a_k}}{\sum_i e^{a_i}}\right)^2 = y_k(1 - y_k)$$

$$\frac{\partial y_k}{\partial a_j} = \frac{-e^{a_k} e^{a_j}}{(\sum_i e^{a_i})^2} = -y_k y_j \text{ for } j \neq k$$

Background

- According to

$$a_{nj} = \mathbf{w}_j^{\mathrm{T}} \phi_n$$

we have

$$\nabla_{\mathbf{w}_j} a_{nj} = \phi_n$$

- Given $\frac{\partial E}{\partial y_{nk}} = -\frac{t_{nk}}{y_{nk}}$ and $\frac{\partial y_k}{\partial a_j} = y_k(I_{kj} - y_j)$, we can compute

$$\frac{\partial E}{\partial a_{nj}} = \sum_{k=1}^{K} \frac{\partial E}{\partial y_{nk}} \frac{\partial y_{nk}}{\partial a_{nj}} = -\sum_{k=1}^{K} \frac{t_{nk}}{y_{nk}} y_{nk}(I_{kj} - y_{nj})$$

$$= -\sum_{k=1}^{K} t_{nk}(I_{kj} - y_{nj}) = -t_{nj} + \sum_{k=1}^{K} t_{nk} y_{nj} = y_{nj} - t_{nj}$$

(1-of-K coding scheme: $\forall n, \sum_k t_{nk} = 1$)

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Newton-Raphson iterative optimization

$\boxed{\mathbf{w} \rightarrow a \rightarrow y \rightarrow E}$

- Gradient

$$\nabla_{\mathbf{w}_j} E(\mathbf{w}_1, \ldots, \mathbf{w}_K) = \sum_{n=1}^{N} \frac{\partial E}{\partial a_{nj}} \nabla_{\mathbf{w}_j} a_{nj} = \sum_{n=1}^{N} (y_{nj} - t_{nj}) \phi_n$$

- Hessian

$$\nabla_{\mathbf{w}_k} \nabla_{\mathbf{w}_j} E(\mathbf{w}_1, \ldots, \mathbf{w}_K) = \sum_{n=1}^{N} y_{nk} (I_{kj} - y_{nj}) \phi_n \phi_n^{\mathrm{T}}$$

- With gradient and Hessian, Newton-Raphson method works

$$\mathbf{w}^{(\mathrm{new})} = \mathbf{w}^{(\mathrm{old})} - \mathbf{H}^{-1} \nabla E(\mathbf{w})$$

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Discriminative approach summary

- Posterior probability and logistic regression

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma\left(\mathbf{w}^{\mathrm{T}}\phi\right) \text{ and } p(\mathcal{C}_2|\phi) = 1 - p(\mathcal{C}_1|\phi)$$

- The negative log likelihood (cross entropy error)

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

- Newton-Raphson method for iterative optimization

$$\mathbf{w}^{(\mathrm{new})} = \mathbf{w}^{(\mathrm{old})} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- It can be extended to multiclass classification

Summary

- Linear discriminant
  - Two-class discriminant
  - K-class discriminant
  - Fisher's linear discriminant
- Probabilistic generative model
  - Class-conditional probability and class prior probability
  - ML solution
- Probabilistic discriminative model: Logistic regression
  - Posterior probability
  - Newton-Raphson iterative optimization

References

- Chapters 4.1, 4.2, and 4.3 in the PRML textbook

Thank You for Your Attention!

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