Linear Discriminant Analysis

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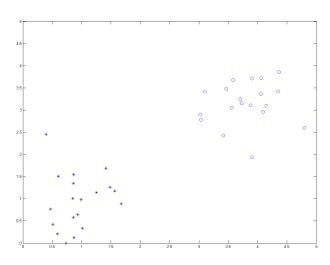
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Agenda

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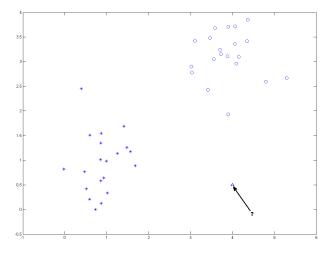
Discriminant analysis

A simple picture



Discriminant analysis

A simple picture



Discriminant analysis

Discriminant analysis

What is the discriminant analysis?

Main goal of the discriminant analysis is a formulation criteria for class separability.

This is a general description of the pattern recognition task – classification problem.

Discriminant function

In discriminant analysis we seek a function that allows class separability. Such function is termed discriminant function.

Discriminant function

In two–class problem, a discriminant function $h(\mathbf{x})$ is a function for which

$$h(\mathbf{x}) \begin{cases} > k, & \Rightarrow \mathbf{x} \in \omega_1 \\ < k, & \Rightarrow \mathbf{x} \in \omega_2 \end{cases} , \tag{1}$$

for constant k, and the pattern \mathbf{x} .

In the case of equality ($h(\mathbf{x} = k)$), the pattern \mathbf{x} may be assigned arbitrarily to one of the two classes.

Discriminant function

Discriminant functions are not unique.

Monotonic function

If function $f(\cdot)$ is a monotonic function then

$$g(\mathbf{x}) = f(h(\mathbf{x})) \begin{cases} > k', & \Rightarrow \mathbf{x} \in \omega_1 \\ < k', & \Rightarrow \mathbf{x} \in \omega_2 \end{cases}.$$

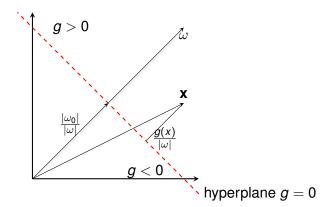
where k' = f(k).

Let us consider the family of discrimiant functions that are linear combinations of the components of $\mathbf{x} = [x_1, x_2, \dots, x_p]^T$, i.e.

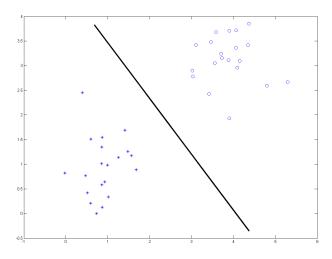
$$g(\mathbf{x}) = \omega^T \mathbf{x} + \omega_0 = \sum_{i=1}^{p} \omega_i x_i + \omega_0.$$
 (2)

A complete specification of a linear discriminant function is achieved by prescribing thw weight wector ω and the treshold weight ω_0 .

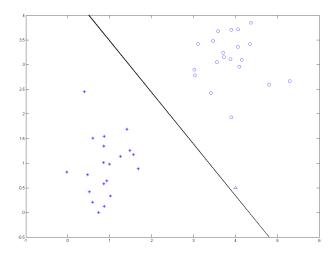
Geometry of linear discrimination function



Geometry of linear discrimination function



Geometry of linear discrimination function



Linear machine

Linear machine

A pattern classifier employing linear discriminant function is termed a linear machine.

Suppose we are given a set of prototype points (vectors) $\mathbf{p}_1,\ldots,\mathbf{p}_c$, one for each of the c classes ω_1,\ldots,ω_c . The minimum–distance classifier assigns a pattern \mathbf{x} to the class ω_k associated with the nearest point \mathbf{p}_k .

For each point, the squared Euclidean distance is

$$d_k = |\mathbf{x} - \mathbf{p}_k|^2$$

Linear machine

Let us consider the squared Euclidean distance

$$d_k = |\mathbf{x} - \mathbf{p}_k|^2 = \mathbf{x}^T \mathbf{x} - 2\mathbf{x}^T \mathbf{p}_k + \mathbf{p}_k^T \mathbf{p}_k.$$

Minimum–distance classification is achieved by comparing the expressions $\mathbf{x}^T \mathbf{p}_k - 1/2 \mathbf{p}_k^T \mathbf{p}_k$ and selecting the largest value. Thus the linear discriminant function is

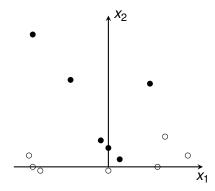
$$g_k(\mathbf{x}) = \omega_k^T \mathbf{x} + \omega_{k,0},$$

where

$$\omega_k = \mathbf{p}_k$$
 $\omega_{k,0} = \frac{1}{2} |\mathbf{p}_k|^2$

Generalised linear discrimination function

Generalised linear discriminant function



Generalised linear discriminant function

A generalised linear discriminant function, also termed a phi machine is a discriminant function of the form

$$g(\mathbf{x}) = \omega^T \phi + \omega_0,$$

where

$$\phi = \begin{bmatrix} \phi_1(\mathbf{x}) \\ \phi_2(\mathbf{x}) \\ \vdots \\ \phi_D(\mathbf{x}) \end{bmatrix}$$

is a vector function of x.

If D = p, and $\phi_i(\mathbf{x}) = x_i$, then we have a linear discriminant function.

Generalised linear discrimination function

Generalised linear discriminant function

Generalised ...

The discriminant function is linear in the functions ϕ_i , not in the original features x_i .

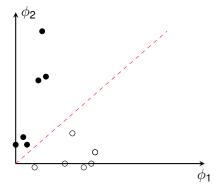
If we make the transformation

$$\phi_1(\mathbf{x}) = x_1^2$$
$$\phi_2(\mathbf{x}) = x_2$$

then the classes in previous example can be separated in the ϕ -space by a straight line.

Generalised linear discrimination function

Generalised linear discriminant function



General ideas

General ideas

Suppose we have a set of training patters $\mathbf{x}_1, \dots, \mathbf{x}_N$, each of which is assigned to one of two classes ω_1 or ω_2 . Using this set we seek a weight vector ω and a treshold ω_0 such that

$$\omega^T \mathbf{x} + \omega_0 \begin{cases} > 0, \\ < 0, \end{cases} \Rightarrow \mathbf{x} \in \begin{cases} \omega_1 \\ \omega_2 \end{cases},$$

General ideas

A discriminant function can be defined in the following way

$$\mathbf{v}^T \mathbf{z} egin{cases} > 0, \\ < 0, \end{cases} \Rightarrow \mathbf{x} \in egin{cases} \omega_1 \\ \omega_2 \end{cases},$$

where

$$\mathbf{z} = \left[1, x_1, \dots, x_p\right]^T,$$

and

$$\mathbf{v} = \left[\omega_0, \omega_1, \ldots, \omega_p\right]^T.$$

z could also be

$$\mathbf{z} = [1, \phi_1(\mathbf{x}), \dots, \phi_D(\mathbf{x})]^T$$

with \mathbf{v} a (D+1)-dimensional vector of weights.

General ideas

A sample in class ω_2 is classified correctly, if

$$\mathbf{v}^T\mathbf{z} < 0$$
.

If we were to redefine all samples in class ω_2 in the design set by their negative values and denote these redefined samples by \mathbf{y} , then we seek a value for \mathbf{v} which satisfies

$$\mathbf{v}^T\mathbf{y} > 0$$
,

for all \mathbf{y}_i corresponding to \mathbf{x}_i in the design set.

$$\mathbf{y}_{i}^{T} = \begin{cases} \begin{bmatrix} 1, \mathbf{x}_{i}^{T} \end{bmatrix}^{T}, & \mathbf{x}_{i} \in \omega_{1} \\ \begin{bmatrix} -1, -\mathbf{x}_{i}^{T} \end{bmatrix}^{T}, & \mathbf{x}_{i} \in \omega_{2} \end{cases}$$

The perceptron criterion function is defined as follows

$$J_{P}(\mathbf{v}) = \sum_{\mathbf{y}_{i} \in Y} \left(-\mathbf{v}^{T} \mathbf{y}_{i} \right),$$

where

$$Y = \left\{ \mathbf{y}_I | \mathbf{v}^T \mathbf{y}_I < 0
ight\}.$$

 J_P is proportional to the sum of the distances of the misclassified samples to the decision boundary.

Error–correction procedure

Since the criterion function J_P is continuous, we can use a gradient–based procedure, such as the method of steepest descent, to determine its minimum

$$\frac{\partial J_P}{\partial \mathbf{v}} = \sum_{\mathbf{y}_i \in Y} (-\mathbf{y}_i)$$

which is the sum of misclassified patterns.

$$\mathbf{v}_{k+1} = \mathbf{v}_k + \rho_k \sum_{\mathbf{y}_i \in Y} \mathbf{y}_i$$

where ρ_k is the scale parameter that determine the step size.

Error–correction procedure

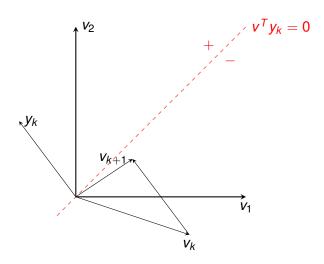
The mentioned algorithm is sometimes referred to as *many–pattern adaptation* or *batch–update* since all given pattern samples are used in the update **v**.

The corresponding *single-pattern adaptation* scheme is

$$\mathbf{v}_{k+1} = \mathbf{v}_k + \rho_k \mathbf{y}_i.$$

where \mathbf{y}_i is a training sample that has been misclassified by \mathbf{v}_k .

Error-correction procedure



Variants

ρ parameter

What is the best value of the scale parameter ρ ?

Constant

For the constant ρ we obtain the *fixed-increment* rule. BTW, is the simplest algorithm for solving systems of linear inequalities.

Variants

ρ parameter

What is the best value of the scale parameter ρ ?

Absolute correction rule

Choose the value of ρ so that the value of

$$\mathbf{v}_{k+1}^T \mathbf{y}_i$$

is positive.

Thus

$$\rho > \frac{\left|\mathbf{v}_{k+1}^{T}\mathbf{y}_{i}\right|}{|\mathbf{y}_{i}|^{2}}$$

where \mathbf{y}_i is misclassified pattern presented at the k-th step.

Variants

Margin b

A margin, b > 0, is introduced and the weight vector is updated whenever

$$\mathbf{v}^T\mathbf{y}_i \leq b.$$

Thus, the solution vector \mathbf{v} must lie at a distance greater than $\frac{b}{|\mathbf{y}_i|}$ from each hyperplane $\mathbf{v}^T\mathbf{y}_i = 0$.

Relaxation algorithm

Relaxation algorithm

The relaxation algorithm or Agmon–Mays algorithm minimises the criterion

$$J_R = \frac{1}{2} \sum_{\mathbf{y}_i \in Y} \frac{\left(\mathbf{v}^T \mathbf{y}_i - b\right)^2}{|\mathbf{y}_i|^2}$$

where Y is $\{\mathbf{y}_i|\mathbf{v}^T\mathbf{y}_i \leq b\}$.

Relaxation algorithm

Relaxation algorithm

Batch update

The basic update formula is

$$\mathbf{v}_{k+1} = \mathbf{v}_k + \rho_k \sum_{\mathbf{y}_i \in Y} \frac{b - \mathbf{v}' \mathbf{y}_i}{|\mathbf{y}_i|^2} \mathbf{y}_i$$

Single-pattern scheme

Single-pattern scheme is defined as follows

$$\mathbf{v}_{k+1} = \mathbf{v}_k + \rho_k \frac{b - \mathbf{v}^T \mathbf{y}_i}{|\mathbf{y}_i|^2} \mathbf{y}_i$$

Fisher's criterion

Fisher's criterion

Fisher's approach

The approach adopted by Fisher was to find a linear combination of the variables that separates the two classes as much as possible. That is, we seek the direction along which the two classes are best separated (in some sense).

Fisher's criterion

The criterion proposed by Fisher is the ratio between–class to within–class variances. We seek a direction **w** such that

$$J_F = \frac{\left|\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)\right|^2}{\mathbf{w}^T S_W \mathbf{w}}$$

is a maximum.

Fisher's criterion

Fisher's criterion

List of parameters:

- m₁, m₂ are the group means,
- ullet S_W is the pooled within–class sample covariance matrix

$$S_W = rac{1}{N-2} \left(N_1 \hat{\Sigma}_1 + N_2 \hat{\Sigma}_2
ight)$$

- $\hat{\Sigma}_1$, $\hat{\Sigma}_2$ are the maximum likelihood estimates of the covariance matrices of classes ω_1 and ω_2 , respectively,
- N_i is number of samples in class ω_i , $(N_1 + N_2 = N)$.

Fisher's criterion

Fisher's criterion

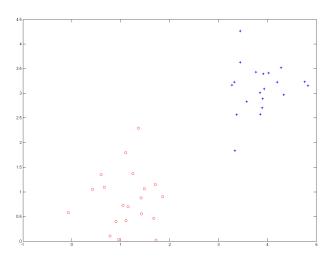
The solution that maximises J_F can be obtained by differentiating J_F with respect to \mathbf{w} and equating to zero. After 25 years, 3 months and 23 days we can obtain the following equation

$$\boldsymbol{w} \propto \mathcal{S}_{W}^{-1} \left(\boldsymbol{m}_{1} - \boldsymbol{m}_{2}\right)$$

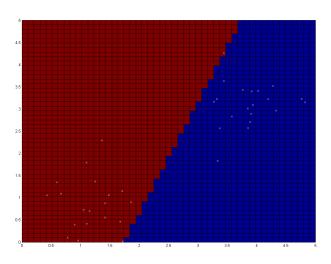
And the assign procedure of pattern \mathbf{x} is given by

$$\left| \boldsymbol{w}^T \boldsymbol{x} - \boldsymbol{w}^T \boldsymbol{m}_1 \right| < \left| \boldsymbol{w}^T \boldsymbol{x} - \boldsymbol{w}^T \boldsymbol{m}_2 \right|.$$

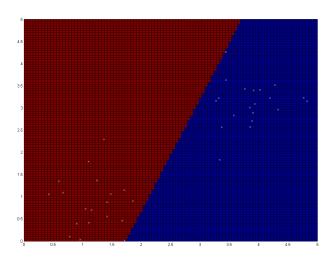
Numerical fun



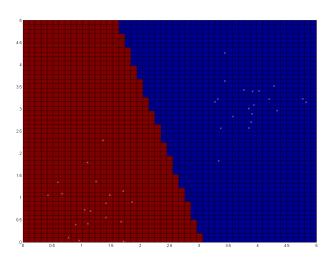
Perceptron



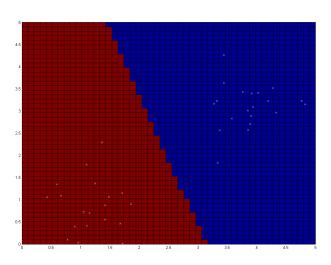
Perceptron



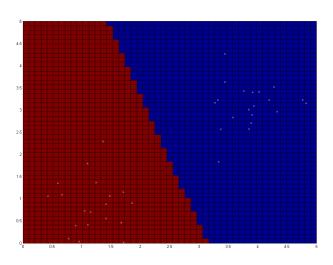
Perceptron



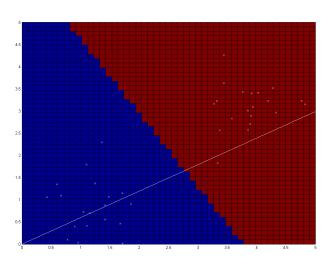
Relaxation



Relaxation



Fisher



Thanks 4 attention

