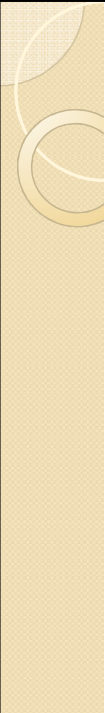


Linear Discriminant Functions

Jacob Hays 5.8, 5.9, 5.11
Amit Pillay
James DeFelice



Minimum Squared Error

- Previous methods only worked on linear separable cases, by looking at misclassified samples to correct error
- MSE looks at all samples, using linear equations to find estimate

Minimum Squared Error

- x space mapped to y space.
- For all samples x_i in dimension d , there exists a y_i of dimension d^\wedge
- Find vector \mathbf{a} making all $\mathbf{a}^t \mathbf{y}_i > 0$
- All samples \mathbf{y}_i in matrix \mathbf{Y} , $\dim n \times d^\wedge$,
- $\mathbf{Y}\mathbf{a} = \mathbf{b}$ (\mathbf{b} is vector of positive constants)

• \mathbf{b} is our margin for error

$$\begin{pmatrix} y_{10} & y_{11} & \dots & y_{1d} \\ y_{20} & y_{21} & \dots & y_{2d} \\ \dots & \dots & \dots & \dots \\ y_{n0} & y_{n1} & \dots & y_{nd} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \cdot \\ a_d \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \dots \\ \dots \\ b_n \end{pmatrix}$$

Minimum Squared Error

- \mathbf{Y} is rectangular ($n \times d^\wedge$), so it does not have a direct inverse to solve $\mathbf{Y}\mathbf{a} = \mathbf{b}$
- $\mathbf{Y}\mathbf{a} - \mathbf{b} = \mathbf{e}$ – gives error, minimize it

• Square error $\|\mathbf{e}\|^2$ $J_s(\mathbf{a}) = \|\mathbf{Y}\mathbf{a} - \mathbf{b}\|^2 = \sum_{i=1}^n (a^t y_i - b_i)^2$

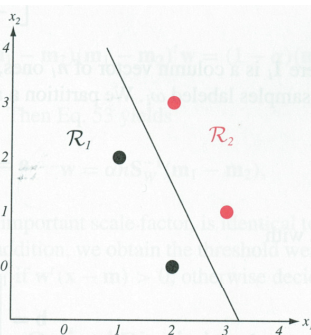
• Take Gradient $\nabla J_s = \sum_{i=1}^n 2(a^t y_i - b_i) y_i = 2\mathbf{Y}^t (\mathbf{Y}\mathbf{a} - \mathbf{b})$

• Gradient should goto Zero $\mathbf{Y}^t \mathbf{Y}\mathbf{a} = \mathbf{Y}^t \mathbf{b}$

Minimum Squared Error

- $\mathbf{Y}^t \mathbf{Y} \mathbf{a} = \mathbf{Y}^t \mathbf{b}$ goes to $\mathbf{a} = (\mathbf{Y}^t \mathbf{Y})^{-1} \mathbf{Y}^t \mathbf{b}$
- $(\mathbf{Y}^t \mathbf{Y})^{-1} \mathbf{Y}^t$ is the psuedo-inverse of \mathbf{Y} , dimension $d \wedge \times n$, can be written as \mathbf{Y}^\dagger
- $\mathbf{Y}^\dagger \mathbf{Y} = \mathbf{I}$ $\mathbf{Y} \mathbf{Y}^\dagger \neq \mathbf{I}$
- $\mathbf{a} = \mathbf{Y}^\dagger \mathbf{b}$ gives us a solution with \mathbf{b} being a margin.

Minimum Squared Error



Four training points and the decision boundary $\mathbf{a}^t \begin{pmatrix} 1 \\ x_1 \\ x_2 \end{pmatrix} = 0$, where \mathbf{a} was found by means of a pseudoinverse technique.

Our matrix \mathbf{Y} is therefore

$$\mathbf{Y} = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 0 \\ -1 & -3 & -1 \\ -1 & -2 & -3 \end{pmatrix}$$

Fisher's Linear Discriminant

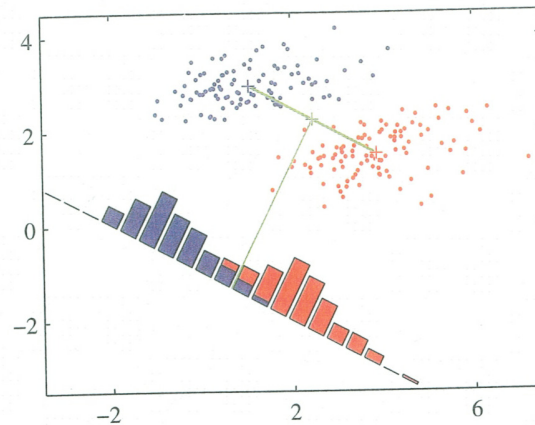
- Based on projection of d-dimensional data onto a line.
- Loses a lot of data, but some orientation of the line might give a good split

$$y = \mathbf{w}^t \mathbf{x}, \quad \|\mathbf{w}\| = 1$$

- y_i is projection of x_i onto line \mathbf{w}
- **Goal:** Find best \mathbf{w} to separate them
- Highly overlapping data performs poorly

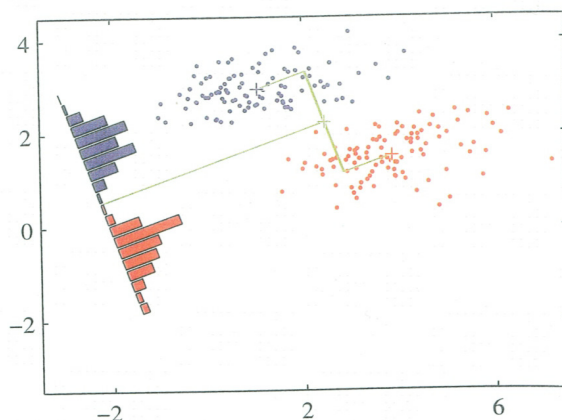
Fisher's Linear Discriminant

- Mean of each class D_i $m_i = \frac{1}{n_i} \sum_{x \in D_i} x$
- $\mathbf{w} = \mathbf{m}_1 - \mathbf{m}_2 / \|\mathbf{m}_1 - \mathbf{m}_2\|$



Fisher's Linear Discriminant

- Scatter Matrices $S_i = \sum_{x \in D_i} (x - m_i)(x - m_i)^t$
- $S_W = S_1 + S_2$ $w = S_W^{-1} (m_1 - m_2)$



Fisher's Relation to MSE

- MSE and Fisher equivalent for specific \mathbf{b}
 - n_i = number of $x \in D_i$
 - $\mathbf{1}_i$ is column vector of n_i full of ones

$$Y = \begin{bmatrix} \mathbf{1}_1 & X_1 \\ -\mathbf{1}_2 & -X_2 \end{bmatrix} \quad a = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix} \quad b = \begin{bmatrix} \frac{n}{n_1} \mathbf{1}_1 \\ \frac{n}{n_2} \mathbf{1}_2 \end{bmatrix}$$

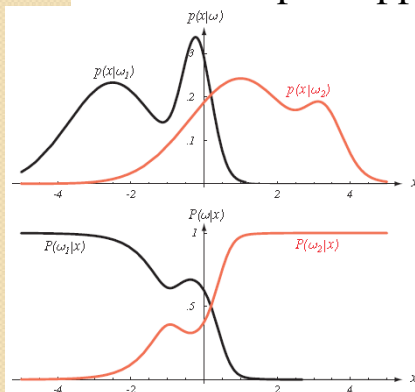
- Plug into $\mathbf{Y}^t \mathbf{Y} \mathbf{a} = \mathbf{Y}^t \mathbf{b}$

$$\begin{bmatrix} \mathbf{1}_1 & -\mathbf{1}_1 \\ X_1' & -X_2' \end{bmatrix} \begin{bmatrix} \mathbf{1}_1 & X_1 \\ -\mathbf{1}_2 & -X_2 \end{bmatrix} \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix} = \begin{bmatrix} \mathbf{1}_1 & -\mathbf{1}_1 \\ X_1' & -X_2' \end{bmatrix} \begin{bmatrix} \frac{n}{n_1} \mathbf{1}_1 \\ \frac{n}{n_2} \mathbf{1}_2 \end{bmatrix}$$

$$w = \alpha n S_W^{-1} (m_1 - m_2)$$

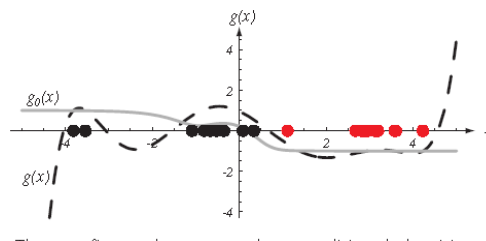
Relation to Optimal Discriminant

- If you set $\mathbf{b} = \mathbf{1}_n$, MSE approaches the optimal Bayes discriminant g_0 as number of samples approaches infinity. (see 5.8.3)



$$g_0(x) = P(\omega_2 | x) - P(\omega_1 | x)$$

$g(x)$ is MSE estimation



Widrow-Hoff / LMS

- LMS – Least Mean Squared
- Still solves when $\mathbf{Y}^t\mathbf{Y}$ is singular

\mathbf{a}, \mathbf{b} , threshold θ , step $\eta(\cdot)$, $\mathbf{k} = 0$

begin

do

$\mathbf{k} = (\mathbf{k} + 1) \bmod n$

$\mathbf{a} = \mathbf{a} + \eta(\mathbf{k})(\mathbf{b}_k - \mathbf{a}^t \mathbf{y}^k) \mathbf{y}^k$

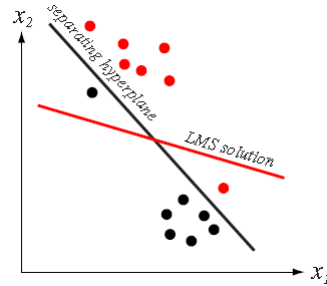
until $|\eta(\mathbf{k})(\mathbf{b}_k - \mathbf{a}^t \mathbf{y}^k)| < \theta$

return \mathbf{a}

end

Widrow-Hoff / LMS

- LMS not guaranteed to converge to a separating plane, even if one exists.



Procedural differences

- Perceptron, relaxation
 - If samples linearly separable, we can find a solution
 - Otherwise, we do not converge to a solution
- MSE
 - Always yields a weight vector
 - May not be the best solution
 - Not guaranteed to be a separating vector

Choosing b

- Arbitrary b, MSE minimizes $\|Ya - b\|^2$
- If linearly separable, we can more smartly choose b
 - Define \hat{a} and β such that
$$Y\hat{a} = \beta > 0$$
 - Every component of β is positive

Modified MSE

- $J_s(a,b) = \|Ya - b\|^2$
- a, b allowed to vary
- Subject to $b > 0$
- Min of J_s is zero
- a that achieves min J_s is the separating vector

Ho-Kashyap/Descent procedure

$$\nabla_a J_s = 2Y^t(Ya - b)$$

$$\nabla_b J_s = -2(Ya - b)$$

- For any b

$$a = Y^\dagger b$$

So, $\nabla_a J_s = 0$ and we're done? **no...**

- Must avoid $b = 0$
- Must avoid $b < 0$

Ho-Kashyap/Descent Procedure

- Pick positive b
- Don't allow reduction of b's components
- Set all positive components of $\nabla_a J_s$ to zero
 - $b(k+1) = b(k) - \eta c$

$$c = \begin{cases} \nabla_b J_s & \text{if } \nabla_b J_s \leq 0 \\ \mathbf{0} & \text{otherwise} \end{cases}$$

$$c = \frac{1}{2} (\nabla_b J_s - |\nabla_b J_s|)$$

Ho-Kashyap/Descent Procedure

$$\nabla_b J_s = -2(Ya - b)$$

$$e = Ya - b$$

$$b_{k+1} = b_k - \eta \frac{1}{2} [\nabla_b J_s - |\nabla_b J_s|]$$

$$b_{k+1} = b_k + 2\eta_k e_k^+$$

$$a_k = Y^\dagger b_k$$

$$e_k^+ = \frac{1}{2}(e_k - |e_k|)$$

Ho-Kashyap

- Algorithm 11
 - Begin initialize $a, b, \eta() < 1$, threshold b_{\min}, k_{\max}
 - do $k = k+1 \text{ mod } n$
 - $e = Ya - b$
 - $e^+ = \frac{1}{2}(e + \text{abs}(e))$
 - $b = b + 2\eta(k)e^+$
 - $a = Y^\dagger b$
 - if $\text{abs}(e) \leq b_{\min}$ then return a, b and exit
 - Until $k = k_{\max}$
 - Print "NO SOLUTION"
 - End
- When $e(k) = 0 \rightarrow$ we have solution
- When $e(k) \leq 0 \rightarrow$ samples not linearly separable

Convergence (separable case)

- If $0 < \eta < 1$, and linearly separable
 - Solution vector exists
 - We will find in finite k steps
- Two possibilities
 - $e(k) = 0$ for some finite k_0
 - No zero in $e()$
- If $e(k_0)$
 - $a(k)$, $b(k)$, $e(k)$ stop changing
 - $Ya(k) = b(k) > 0$ for all $k > k_0$
 - If we find k_0 , algorithm terminates with solution vector

Convergence (separable)

- $e()$ never zero for finite k
- If samples are linearly separable
 - $Ya = b$, $b > 0$
- Because b is positive, either
 - $e(k)$ is zero, or
 - $e(k)$ is positive
- Since $e(k)$ cannot be zero (first bullet), it must be positive

Convergence (separable)

- $\frac{1}{4}(\|e_k\|^2 - \|e_{k+1}\|^2) = \eta(1 - \eta)\|e_k^+\|^2 + \eta^2 e_k^{+t} Y Y^\dagger e_k^+$
 - $Y Y^\dagger$ is symmetric, positive semi-definite
 - $0 < \eta < 1$
- Therefore, $\|e_k\|^2 > \|e_{k+1}\|^2$ if $0 < \eta < 1$
 - $\|e\|$ will eventually converge to zero
 - a will eventually converge to solution vector

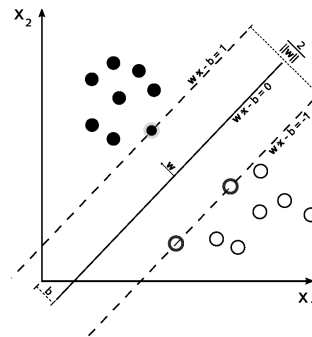
Convergence (non-separable)

- If not linearly separable, may obtain a non-zero error vector without positive components
- Still have
 - $\frac{1}{4}(\|e_k\|^2 - \|e_{k+1}\|^2) = \eta(1 - \eta)\|e_k^+\|^2 + \eta^2 e_k^{+t} Y Y^\dagger e_k^+$
 - So limiting $\|e\|$ cannot be zero
 - Will converge to a non-zero value
- Convergence says that
 - $e_k^+ = 0$ for some finite k (separable)
 - e_k^+ will converge to zero while $\|e\|$ is bounded away from zero (non-separable)

Support Vector Machines (SVMs)

SVMs

- Representing data in higher dimensions space, SVM will construct a separating hyperplane in that space, one which maximizes margin between the two data sets.



Application

- Face detection, verification, and recognition
- Object detection and recognition
- Handwritten character and digit recognition
- Text detection and categorization
- Speech and speaker verification, recognition
- Information and image retrieval

Formalization

- We are given some training data, a set of points of the form

$$\mathcal{D} = \{(\mathbf{x}_i, c_i) \mid \mathbf{x}_i \in \mathbb{R}^p, c_i \in \{-1, 1\}\}_{i=1}^n$$

Equation of separating hyperplane:

$$\mathbf{w} \cdot \mathbf{x} - b = 0.$$

The vector \mathbf{w} is a normal vector. The parameter $b/\|\mathbf{w}\|$ determines the offset of the hyperplane from the origin along the normal vector

Formalization cont...

- Defining two hyperplanes given by equations:

$$\text{H1: } \quad \mathbf{w} \cdot \mathbf{x} - b = 1$$

$$\text{H2: } \quad \mathbf{w} \cdot \mathbf{x} - b = -1.$$

- These hyperplanes are defined in such a way that no points lies between them
- To prevent data points falling between these hyperplanes, following two constraints are defined:

$$\mathbf{w} \cdot \mathbf{x}_i - b \geq 1$$

$$\mathbf{w} \cdot \mathbf{x}_i - b \leq -1$$

Formulation cont...

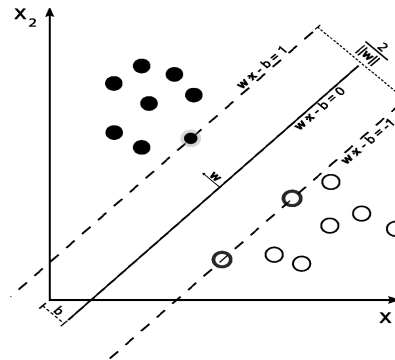
- This can be rewritten as:

$$c_i(\mathbf{w} \cdot \mathbf{x}_i - b) \geq 1, \quad \text{for all } 1 \leq i \leq n$$

- So the formulation of the optimization problem is
 - Choose \mathbf{w} , \mathbf{b} to minimize $\|\mathbf{w}\|$
 subject to

$$c_i(\mathbf{w} \cdot \mathbf{x}_i - b) \geq 1, \quad \text{for all } 1 \leq i \leq n$$

SVM Hyperplane Example



SVM Training

- Lagrange Optimization problem
- Reformulated Optimization Problem is given as:

$$L_P \equiv \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^l \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{w} + b) + \sum_{i=1}^l \alpha_i$$

- Thus the new optimization problem is to minimize L_P w.r.t \mathbf{w} and \mathbf{b} subject to:

$$\alpha_i \geq 0$$

SVM Training cont...

- Dual of Lagrange formulation

The dual of Lagrange states that the gradient descent of L_P with respect to \mathbf{w} and \mathbf{b} vanishes.

so we have the dual as:

$$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

The optimization problem w.r.t dual is to maximize L_D subject to:

$$\alpha_i \geq 0$$

- From the above optimization equation we have:

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

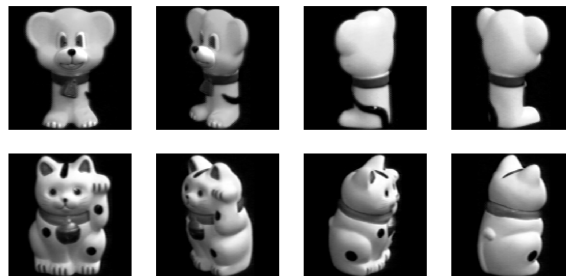
- This shows that the solution is the inner product of input points
- Most of the points have α to be zero and for those points for which α is not zero are the closest points to the separating hyperplane. These points are called support vectors.

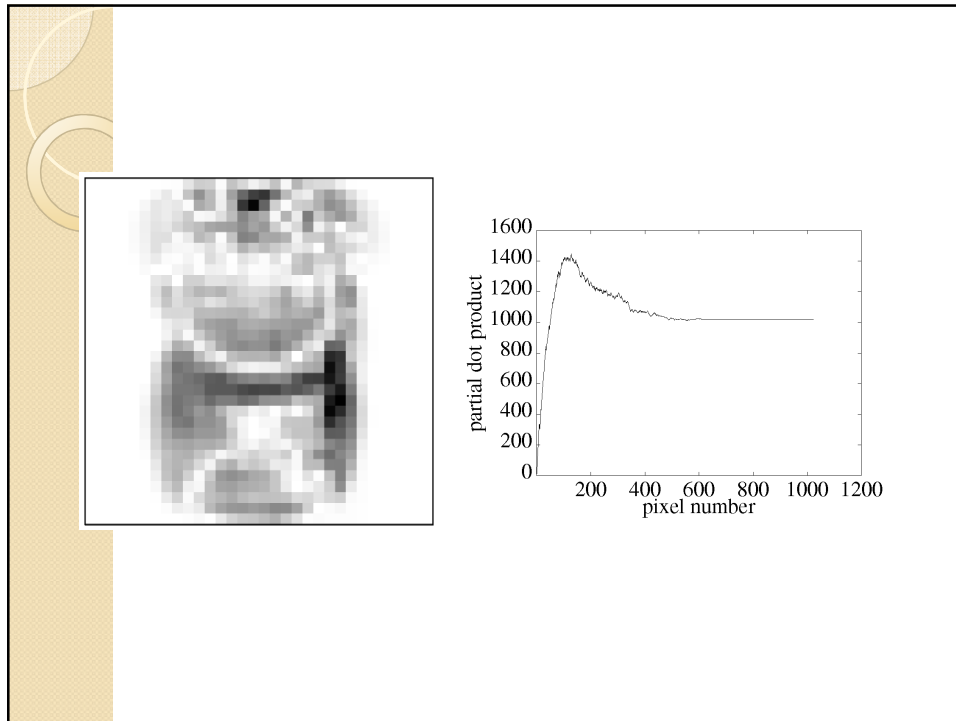
Advantages & Disadvantages of SVM

- Advantages
 - Gives high generalization performance
 - Complexity of SVM classifier is characterized by number of support vectors rather than the dimensionality of transformed space.
- Disadvantages
 - The training time scales somewhere between quadratic and cubic with respect to the number of training samples

Recognition of 3D-Objects

- Experiment involved recognition of 3D objects from the COIL db
- Each coil image is transformed into eight-bit vector of $32 \times 32 = 1024$ components





References

- Pontil, M.; Verri, A., "*Support vector machines for 3D object recognition*," Pattern Analysis and Machine Intelligence, IEEE Transactions Vol. 20, Issue 6, June 1998, pp. 637 – 646
- Christopher J. C. Burges, "*A tutorial on support vector machines for pattern recognition*" (1998)
- R.O. Duda, P. E. Hart and D. Stork, Wiley, *Pattern Classification* (2nd Edition) by 2001
- R.J. Schalkoff. (1992) *Pattern Recognition: Statistical, Structural, and Neural Approaches*, Wiley.*