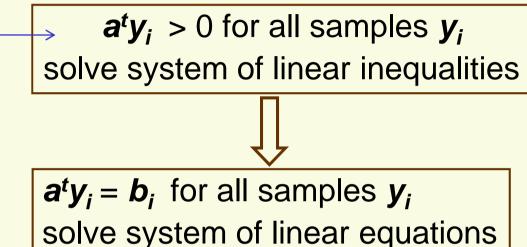
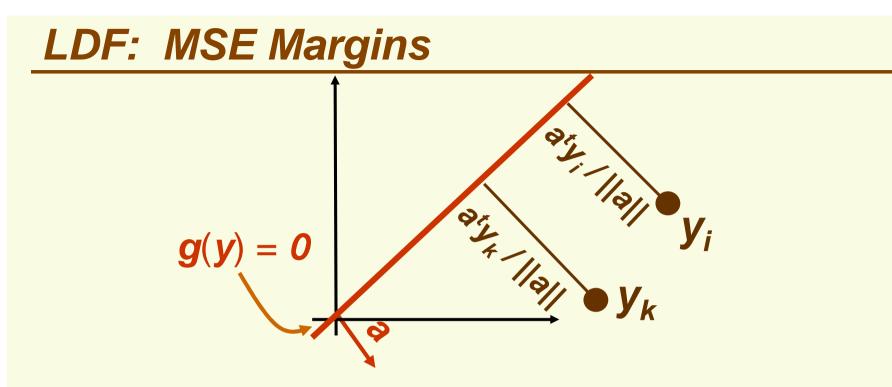
Minimum Squared Error

Idea: convert to easier and better understood problem





- MSE procedure
 - Choose positive constants b₁, b₂,..., b_n
 - try to find weight vector \mathbf{a} s.t. $\mathbf{a}^t \mathbf{y}_i = \mathbf{b}_i$ for all samples \mathbf{y}_i
 - If we can find weight vector a such that a^ty_i = b_i for all samples y_i, then a is a solution because b_i's are positive
 - consider all the samples (not just the misclassified ones)



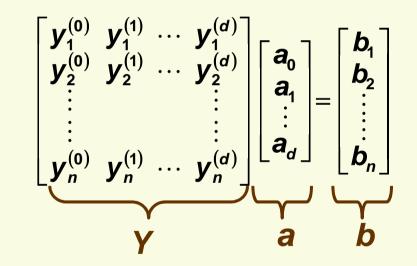
- Since we want a^ty_i = b_i, we expect sample y_i to be at distance b_i from the separating hyperplane (normalized by ||a||)
- Thus b₁, b₂,..., b_n give relative expected distances or "margins" of samples from the hyperplane
- Should make b_i small if sample i is expected to be near separating hyperplane, and make b_i larger otherwise
- In the absence of any additional information, there are good reasons to set b₁ = b₂ = ... = b_n = 1

LDF: MSE Matrix Notation

Need to solve *n* equations

$$\begin{bmatrix} \mathbf{a}^t \mathbf{y}_1 = \mathbf{b}_1 \\ \vdots \\ \mathbf{a}^t \mathbf{y}_n = \mathbf{b}_n \end{bmatrix}$$

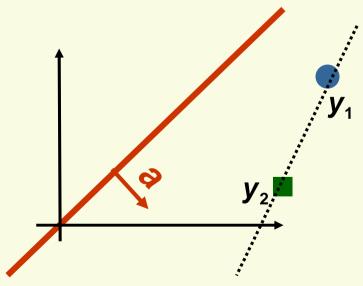
Introduce matrix notation:



Thus need to solve a linear system Ya = b

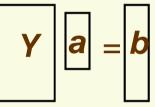
LDF: Exact Solution is Rare

- Thus need to solve a linear system Ya = b
 - Y is an n by (d +1) matrix
- Exact solution can be found only if Y is nonsingular and square, in which case the inverse Y¹ exists
 - $a = Y^1 b$
 - (number of samples) = (number of features + 1)
 - almost never happens in practice
 - in this case, guaranteed to find the separating hyperplane



LDF: Approximate Solution

- Typically Y is overdetermined, that is it has more rows (examples) than columns (features)
 - If it has more features than examples, should reduce dimensionality



- Need Ya = b, but no exact solution exists for an overdetermined system of equation
 - More equations than unknowns
- Find an approximate solution *a*, that is Ya ≈ b
 - Note that approximate solution *a does not* necessarily give the separating hyperplane in the separable case
 - But hyperplane corresponding to *a* may still be a good solution, especially if there is no separating hyperplane

LDF: MSE Criterion Function

 Minimum squared error approach: find *a* which minimizes the length of the error vector *e*

b Ya

- Thus minimize the minimum squared error criterion function: $J_{s}(a) = \|Ya - b\|^{2} = \sum_{i=1}^{n} (a^{t}y_{i} - b_{i})^{2}$
- Unlike the perceptron criterion function, we can optimize the minimum squared error criterion function analytically by setting the gradient to *0*

LDF: Optimizing $J_s(a)$

$$J_{s}(a) = ||Ya - b||^{2} = \sum_{i=1}^{n} (a^{t}y_{i} - b_{i})^{2}$$

Let's compute the gradient:

$$\nabla J_{s}(a) = \begin{bmatrix} \frac{\partial J_{s}}{\partial a_{0}} \\ \vdots \\ \frac{\partial J_{s}}{\partial a_{d}} \end{bmatrix} = 2Y^{t}(Ya - b)$$

Setting the gradient to 0:

$$2Y^{t}(Ya - b) = 0 \implies Y^{t}Ya = Y^{t}b$$

LDF: Pseudo Inverse Solution

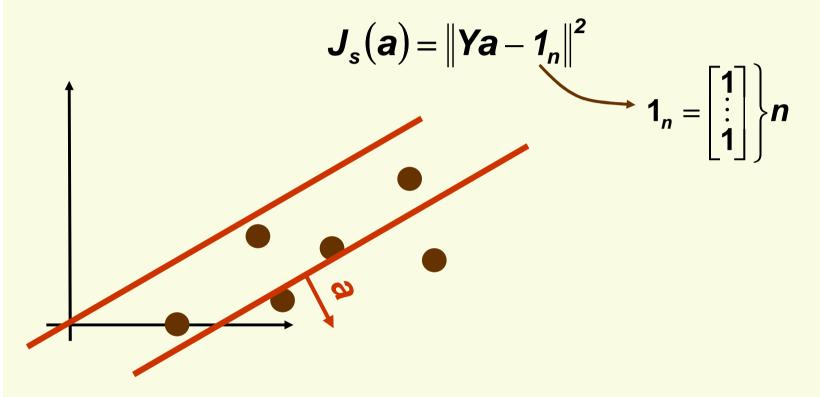
- Matrix Y^tY is square (it has d+1 rows and columns) and it is often non-singular
- If Y^tY is non-singular, its inverse exists and we can solve for a uniquely:

$$\boldsymbol{a} = \left(\boldsymbol{Y}^{t}\boldsymbol{Y}\right)^{-1}\boldsymbol{Y}^{t}\boldsymbol{b}$$

pseudo inverse of Y

 $\left(\left(\mathbf{Y}^{t} \mathbf{Y} \right)^{-1} \mathbf{Y}^{t} \right) \mathbf{Y} = \left(\mathbf{Y}^{t} \mathbf{Y} \right)^{-1} \left(\mathbf{Y}^{t} \mathbf{Y} \right) = \mathbf{I}$

If b₁=...=b_n=1, MSE procedure is equivalent to finding a hyperplane of best fit through the samples y₁,...,y_n



 Then we shift this line to the origin, if this line was a good fit, all samples will be classified correctly

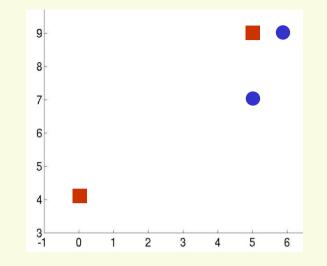
Only guaranteed the separating hyperplane if Ya > 0

• that is if all elements of vector $\mathbf{Y} \mathbf{a} = \begin{bmatrix} \mathbf{a}^t \mathbf{y}_1 \\ \vdots \\ \mathbf{a}^t \mathbf{y}_n \end{bmatrix}$ are positive

- We have Ya ≈ b
- That is $Y_a = \begin{bmatrix} b_1 + \varepsilon_1 \\ \vdots \\ b_n + \varepsilon_n \end{bmatrix}$ where ε may be negative
 - If $\varepsilon_1, \ldots, \varepsilon_n$ are small relative to b_1, \ldots, b_n , then each element of Ya is positive, and a gives a separating hyperplane
 - If approximation is not good, ε_i may be large and negative, for some *i*, thus $b_i + \varepsilon_i$ will be negative and *a* is not a separating hyperplane
- Thus in linearly separable case, least squares solution a does not necessarily gives separating hyperplane
- But it will give a "reasonable" hyperplane

- We are free to choose b. May be tempted to make b large as a way to insure Ya ≈ b > 0
- Does not work
 - Let β be a scalar, let's try βb instead of b
 - if a^* is a least squares solution to Ya = b, then for any scalar β , least squares solution to $Ya = \beta b$ is βa^* $arg min ||Ya - \beta b||^2 = arg min \beta^2 ||Y(a/\beta) - b||^2$ $= arg min ||Y(a/\beta) - b||^2 = \beta a^*$
 - thus if for some *i*th element of *Ya* is less than 0, that is $y_i^t a < 0$, then $y_i^t (\beta a) < 0$,
- Relative difference between components of *b* matters, but not the size of each individual component

- Class 1: (6 9), (5 7)
- Class 2: (5 9), (0 4)
- Set vectors y₁, y₂, y₃, y₄ by adding extra feature and "normalizing"



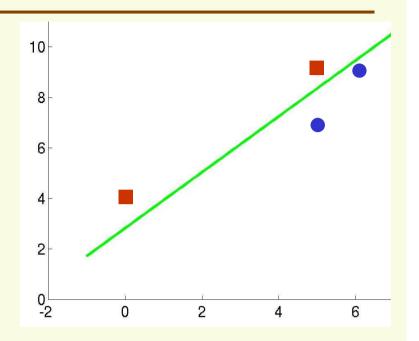
$$\boldsymbol{y}_1 = \begin{bmatrix} \boldsymbol{1} \\ \boldsymbol{6} \\ \boldsymbol{9} \end{bmatrix} \quad \boldsymbol{y}_2 = \begin{bmatrix} \boldsymbol{1} \\ \boldsymbol{5} \\ \boldsymbol{7} \end{bmatrix} \quad \boldsymbol{y}_3 = \begin{bmatrix} -\boldsymbol{1} \\ -\boldsymbol{5} \\ -\boldsymbol{9} \end{bmatrix} \quad \boldsymbol{y}_4 = \begin{bmatrix} -\boldsymbol{1} \\ \boldsymbol{0} \\ -\boldsymbol{4} \end{bmatrix}$$

Matrix Y is then

$$\mathbf{Y} = \begin{bmatrix} 1 & 6 & 9 \\ 1 & 5 & 7 \\ -1 & -5 & -9 \\ -1 & 0 & -4 \end{bmatrix}$$



- Choose $b = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$
- In matlab, $a = Y \setminus b$ solves the least squares problem $a = \begin{bmatrix} 2.7 \\ 1.0 \\ -0.9 \end{bmatrix}$

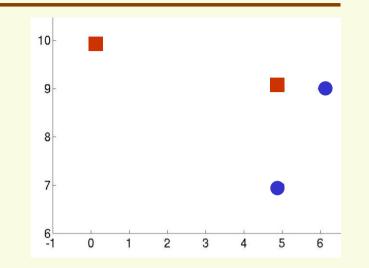


Note *a* is an approximation to *Ya* = *b*, since no exact solution exists
 [0.4]

$$\mathbf{Ya} = \begin{bmatrix} 0.4 \\ 1.3 \\ 0.6 \\ 1.1 \end{bmatrix} \neq \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

This solution does give a separating hyperplane since Ya > 0

- Class 1: (6 9), (5 7)
- Class 2: (5 9), (0 10)
- The last sample is very far compared to others from the separating hyperplane

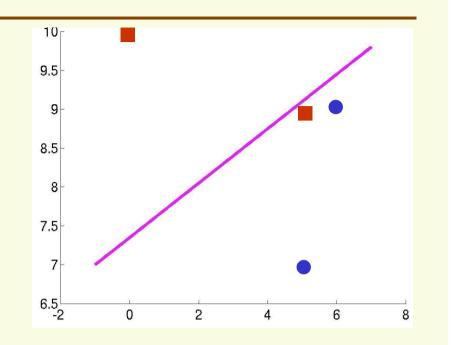


$$y_{1} = \begin{bmatrix} 1\\6\\9 \end{bmatrix} \quad y_{2} = \begin{bmatrix} 1\\5\\7 \end{bmatrix} \quad y_{3} = \begin{bmatrix} -1\\-5\\-9 \end{bmatrix} \quad y_{4} = \begin{bmatrix} -1\\0\\-10 \end{bmatrix}$$

Matrix $Y = \begin{bmatrix} 1&6&9\\1&5&7\\-1&-5&-9\\-1&0&-10 \end{bmatrix}$

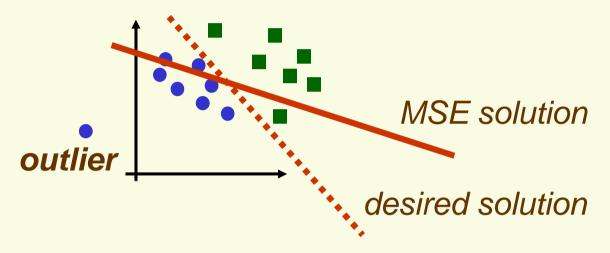


- Choose $b = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$
- In matlab, $a = Y \setminus b$ solves the least squares problem $a = \begin{bmatrix} 3.2 \\ 0.2 \\ -0.4 \end{bmatrix}$



- Note **a** is an approximation to Ya = b, since no exact solution exists $Ya = \begin{bmatrix} 0.2 \\ 0.9 \\ -0.04 \\ 1.16 \end{bmatrix} \neq \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$
- This solution does not give a separating hyperplane since a^ty₃ < 0

 MSE pays to much attention to isolated "noisy" examples (such examples are called outliers)

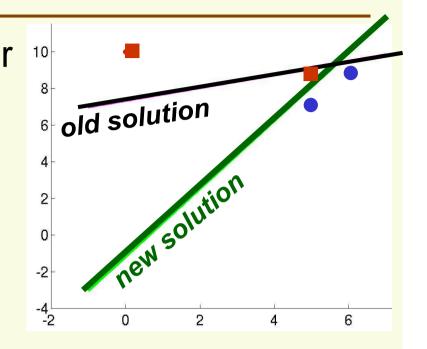


No problems with convergence though, and solution it gives ranges from reasonable to good

- we know that 4th point is far far from separating hyperplane
 - In practice we don't know this
- Thus appropriate $b = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$
- In Matlab, solve a=Y h $a = \begin{bmatrix} -1.1 \\ 1.7 \\ -0.9 \end{bmatrix}$
- Note a is an approximation to Ya = b, Ya =

$$\begin{bmatrix} 0.9\\ 1.0\\ 0.8\\ 10.0 \end{bmatrix} \neq \begin{bmatrix} 1\\ 1\\ 1\\ 10 \end{bmatrix}$$

This solution does give the separating hyperplane since Ya > 0



LDF: Gradient Descent for MSE solution

$$\boldsymbol{J}_{s}(\boldsymbol{a}) = \|\boldsymbol{Y}\boldsymbol{a} - \boldsymbol{b}\|^{2}$$

- May wish to find MSE solution by gradient descent:
 - 1. Computing the inverse of Y^tY may be too costly
 - Y^tY may be close to singular if samples are highly correlated (rows of Y are almost linear combinations of each other)
 - computing the inverse of Y^tY is not numerically stable
- In the beginning of the lecture, computed the gradient:

 $\nabla J_{s}(a) = 2Y^{t}(Ya - b)$

LDF: Widrow-Hoff Procedure

$$\nabla \boldsymbol{J}_{s}(\boldsymbol{a}) = \boldsymbol{2} \boldsymbol{Y}^{t} (\boldsymbol{Y} \boldsymbol{a} - \boldsymbol{b})$$

• Thus the update rule for gradient descent: $\boldsymbol{a}^{(k+1)} = \boldsymbol{a}^{(k)} - \eta^{(k)} \boldsymbol{Y}^{t} (\boldsymbol{Y} \boldsymbol{a}^{(k)} - \boldsymbol{b})$

- If η^(k) = η⁽¹⁾ / k weight vector a^(k) converges to the MSE solution a, that is Y^t(Ya-b)=0
- Widrow-Hoff procedure reduces storage requirements by considering single samples sequentially:

$$\boldsymbol{a}^{(k+1)} = \boldsymbol{a}^{(k)} - \eta^{(k)} \boldsymbol{y}_i \left(\boldsymbol{y}_i^t \boldsymbol{a}^{(k)} - \boldsymbol{b}_i \right)$$

- In the MSE procedure, if b is chosen arbitrarily, finding separating hyperplane is not guaranteed
- Suppose training samples are linearly separable. Then there is **a**^s and positive **b**^s s.t.

 $Ya^{s} = b^{s} > 0$

- If we knew b^s could apply MSE procedure to find the separating hyperplane
- Idea: find both a^s and b^s
- Minimize the following criterion function, restricting to positive **b**:

$$J_{HK}(a,b) = \|Ya - b\|^2$$

$$J_{HK}(a,b) = \|Ya - b\|^2$$

As usual, take partial derivatives w.r.t. a and b

$$\nabla_{a}J_{HK} = 2Y^{t}(Ya - b) = 0$$
$$\nabla_{b}J_{HK} = -2(Ya - b) = 0$$

- Use modified gradient descent procedure to find a minimum of J_{HK}(a,b)
- Alternate the two steps below until convergence:
 1) Fix *b* and minimize *J_{HK}(a,b)* with respect to *a* 2) Fix *a* and minimize *J_{HK}(a,b)* with respect to *b*

$$\nabla_a J_{HK} = 2Y^t (Ya - b) = 0 \qquad \nabla_b J_{HK} = -2(Ya - b) = 0$$

Alternate the two steps below until convergence:

- 1) Fix **b** and minimize $J_{HK}(a, b)$ with respect to **a**
- 2) Fix **a** and minimize $J_{HK}(a, b)$ with respect to **b**
- Step (1) can be performed with pseudoinverse
 - For fixed *b* minimum of *J_{HK}*(*a*,*b*) with respect to *a* is found by solving

 $\mathbf{2}\mathbf{Y}^{t}(\mathbf{Y}\mathbf{a}-\mathbf{b})=\mathbf{0}$

Thus

$$\boldsymbol{a} = \left(\mathbf{Y}^t \mathbf{Y} \right)^{-1} \mathbf{Y}^t \boldsymbol{b}$$

- Step 2: fix **a** and minimize **J_{HK}**(**a**, **b**) with respect to **b**
- We can't use b = Ya because b has to be positive
- Solution: use modified gradient descent
- start with positive b, follow negative gradient but refuse to decrease any components of b
- This can be achieved by setting all the positive components of \(\nabla_b J\) to \(\mathcal{O}\)
- Not doing steepest descent anymore, but we are still doing descent and ensure that b is positive

The Ho-Kashyap procedure:

0) Start with arbitrary $a^{(1)}$ and $b^{(1)} > 0$, let k = 1

```
repeat steps (1) through (4)
```

1)
$$e^{(k)} = Ya^{(k)} - b^{(k)}$$

2) Solve for
$$\boldsymbol{b}^{(k+1)}$$
 using $\boldsymbol{a}^{(k)}$ and $\boldsymbol{b}^{(k)}$
 $\boldsymbol{b}^{(k+1)} = \boldsymbol{b}^{(k)} + \eta \left[\mathbf{e}^{(k)} + |\mathbf{e}^{(k)}| \right]$

3) Solve for
$$a^{(k+1)}$$
 using $b^{(k+1)}$
 $a^{(k+1)} = (Y^{t}Y)^{-1}Y^{t}b^{(k+1)}$

4)
$$k = k + 1$$

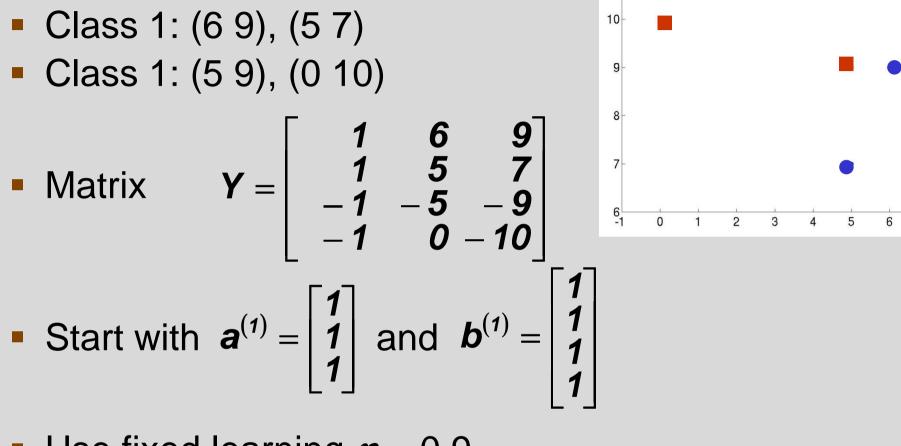
until $e^{(k)} \ge 0$ or $k \ge k_{max}$ or $b^{(k+1)} = b^{(k)}$

• For convergence, learning rate should be fixed between $0 < \eta < 1$

- In the linearly separable case,
 - $e^{(k)} = 0$, found solution, stop
 - one of components of $e^{(k)}$ is positive, algorithm continues

- In non separable case,
 - *e*^(k) will have only negative components eventually, thus found proof of nonseparability
 - No bound on how many iteration need for the proof of nonseparability

LDF: Ho-Kashyap Procedure Example



- Use fixed learning $\eta = 0.9$
- At the start $Ya^{(1)} = \begin{bmatrix} 16\\ 13\\ -15\\ -11 \end{bmatrix}$

LDF: Ho-Kashyap Procedure Example

Iteration 1:

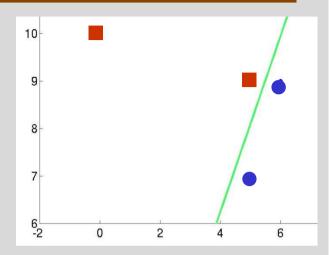
•
$$\mathbf{e}^{(1)} = \mathbf{Y}\mathbf{a}^{(1)} - \mathbf{b}^{(1)} = \begin{bmatrix} \mathbf{16} \\ \mathbf{13} \\ -\mathbf{15} \\ -\mathbf{11} \end{bmatrix} - \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \\ \mathbf{1} \\ \mathbf{1} \end{bmatrix} = \begin{bmatrix} \mathbf{15} \\ \mathbf{12} \\ -\mathbf{16} \\ -\mathbf{12} \end{bmatrix}$$

solve for
$$b^{(2)}$$
 using $a^{(1)}$ and $b^{(1)}$
 $b^{(2)} = b^{(1)} + 0.9[e^{(1)} + e^{(1)}] = \begin{bmatrix} 1\\1\\1\\1 \end{bmatrix} + 0.9\begin{bmatrix} 15\\12\\-16\\-12 \end{bmatrix} + \begin{bmatrix} 15\\12\\16\\12 \end{bmatrix} = \begin{bmatrix} 28\\22.6\\1\\1 \end{bmatrix}$

$$\boldsymbol{a}^{(2)} = (\boldsymbol{Y}^{t} \boldsymbol{Y})^{-1} \boldsymbol{Y}^{t} \boldsymbol{b}^{(2)} = \begin{bmatrix} -2.6 & 4.7 & 1.6 & -0.5 \\ 0.16 & -0.1 & -0.1 & 0.2 \\ 0.26 & -0.5 & -0.2 & -0.1 \end{bmatrix} * \begin{bmatrix} 28 \\ 22.6 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 34.6 \\ 2.7 \\ -3.8 \end{bmatrix}$$

LDF: Ho-Kashyap Procedure Example

- Continue iterations until Ya > 0
 - In practice, continue until minimum component of *Ya* is less then 0.01



After 104 iterations converged to solution

$$a = \begin{bmatrix} -34.9 \\ 27.3 \\ -11.3 \end{bmatrix} \qquad b = \begin{bmatrix} 28 \\ 23 \\ 1 \\ 147 \end{bmatrix}$$

a does gives a separating hyperplane

$$Ya = \begin{bmatrix} 27.2 \\ 22.5 \\ 0.14 \\ 1.48 \end{bmatrix}$$

- Suppose we have *m* classes
- Define *m* linear discriminant functions

$$g_i(x) = w_i^t x + w_{i0}$$
 $i = 1,...,m$

- Given \boldsymbol{x} , assign class \boldsymbol{c}_i if $\boldsymbol{g}_i(\boldsymbol{x}) \ge \boldsymbol{g}_j(\boldsymbol{x}) \qquad \forall \mathbf{j} \neq \mathbf{i}$
- Such classifier is called a *linear machine*
- A linear machine divides the feature space into c decision regions, with g_i(x) being the largest discriminant if x is in the region R_i

- For each class *i*, find weight vector \boldsymbol{a}_i , s.t. $\begin{cases} \boldsymbol{a}_i^t \boldsymbol{y} = 1 & \forall \boldsymbol{y} \in \textbf{class i} \\ \boldsymbol{a}_i^t \boldsymbol{y} = 0 & \forall \boldsymbol{y} \notin \textbf{class i} \end{cases}$
- Let Y_i be matrix whose rows are samples from class i, so it has d+1 columns and n_i rows
- Let's pile all samples in *n* by *d* + 1 matrix *Y*:

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \\ \vdots \\ \mathbf{Y}_m \end{bmatrix} = \begin{bmatrix} sample from \ class1 \\ sample from \ class1 \\ \vdots \\ sample from \ class m \\ sample from \ class m \end{bmatrix}$$

Let b_i be a column vector of length n which is 0 everywhere except rows corresponding to samples from class i, where it is 1: [0]

$$\boldsymbol{b}_{i} = \left| \begin{array}{c} 1\\1\\1\\1\\0\\0 \end{array} \right|^{2} \text{ rows corresponding to samples from class i}$$

- Let's pile all \boldsymbol{b}_i as columns in \boldsymbol{n} by \boldsymbol{c} matrix \boldsymbol{B} $\boldsymbol{B} = [\boldsymbol{b}_1 \cdots \boldsymbol{b}_n]$
- Let's pile all a_i as columns in d+1 by m matrix A

$$\mathbf{W} = \begin{bmatrix} \mathbf{a}^1 & \cdots & \mathbf{a}^m \end{bmatrix} = \begin{bmatrix} \mathbf{a}^1 & \cdots & \mathbf{a}^m \\ \mathbf{w} = \mathbf{a}^n & \mathbf{a}^n \\ \mathbf{w} = \mathbf{a}^n & \mathbf{a}^n \end{bmatrix}$$

m LSE problems can be represented in *YA* = *B*:

 $\begin{bmatrix} sample from \ class1 \\ sample from \ class2 \\ sample from \ class3 \\ sample from \ clas$

Our objective function is:

$$J(\mathbf{A}) = \sum_{i=1}^{m} \|\mathbf{Y}\mathbf{a}_i - \mathbf{b}_i\|^2$$

• J(A) is minimized with the use of pseudoinverse $A = (Y^{t}Y)^{-1}YB$

LDF: Summary

Perceptron procedures

- find a separating hyperplane in the linearly separable case,
- do not converge in the non-separable case
- can force convergence by using a decreasing learning rate, but are not guaranteed a reasonable stopping point

MSE procedures

- converge in separable and not separable case
- may not find separating hyperplane if classes are linearly separable
- use pseudoinverse if Y'Y is not singular and not too large
- use gradient descent (Widrow-Hoff procedure) otherwise

Ho-Kashyap procedures

- always converge
- find separating hyperplane in the linearly separable case
- more costly