CS4442/9542b Artificial Intelligence II prof. Olga Veksler

Lecture 4
Machine Learning
Linear Classifier

Outline

- Optimization with gradient descent
- Linear Classifier
 - Two classes
 - Multiple classes
 - Perceptron Criterion Function
 - Batch perceptron rule
 - Single sample perceptron rule
 - Minimum Squared Error (MSE) rule
 - Pseudoinverse

Optimization

• How to minimize a function of a single variable $J(x) = (x-5)^2$

From calculus, take derivative, set it to 0

$$\frac{d}{dx}J(x)=0$$

- Solve the resulting equation
 - maybe easy or hard to solve
- Example above is easy:

$$\frac{d}{dx}J(x)=2(x-5)=0 \implies x=5$$

Optimization

How to minimize a function of many variables

$$J(\mathbf{x}) = J(\mathbf{x}_1, ..., \mathbf{x}_d)$$

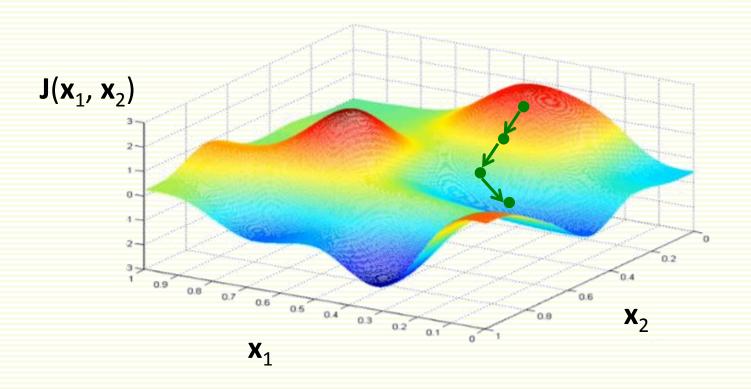
From calculus, take partial derivatives, set them to 0

gradient

$$\begin{bmatrix} \frac{\partial}{\partial x_1} J(x) \\ \vdots \\ \frac{\partial}{\partial x_d} J(x) \end{bmatrix} = \nabla J(x) = 0$$

- Solve the resulting system of d equations
- It may not be possible to solve the system of equations above analytically

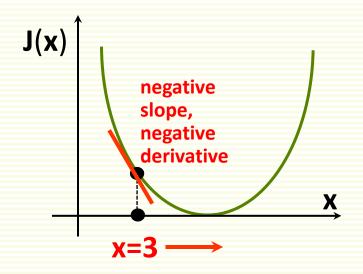
Optimization: Gradient Direction

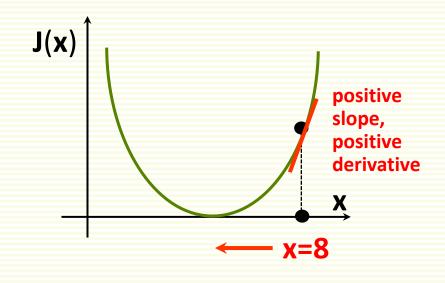


- Gradient $\nabla J(x)$ points in the direction of steepest increase of function J(x)
- $-\nabla J(x)$ points in the direction of steepest decrease

Gradient Direction in 1D

- Gradient is just derivative in 1D
- Example: $J(x) = (x-5)^2$ and derivative is $\frac{d}{dx}J(x) = 2(x-5)$





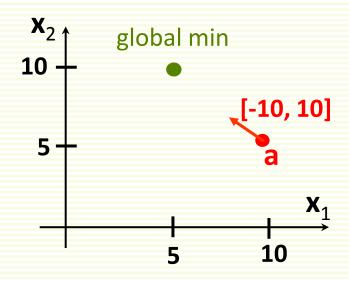
- Let x = 3
- $\bullet \quad -\frac{d}{dx}J(3)=4$
- derivative says increase x

$$\bullet \quad -\frac{d}{dx}J(3)=-6$$

derivative says decrease x

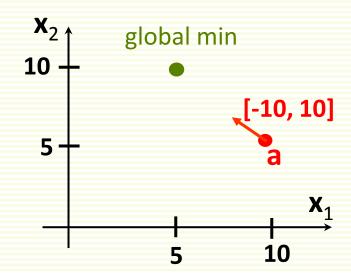
Gradient Direction in 2D

- $J(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 5)^2 + (\mathbf{x}_2 10)^2$
- $\frac{\partial}{\partial x_{1}} J(x) = 2(x_{1} 5)$ $\frac{\partial}{\partial x_{2}} J(x) = 2(x_{2} 10)$
- Let **a** = [10, 5]
- $\frac{\partial}{\partial x_1} J(a) = -10$
- $-\frac{\partial}{\partial x_2}J(a)=10$



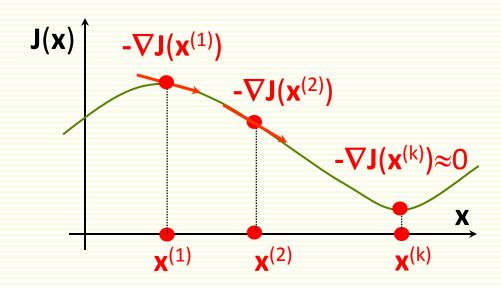
Gradient Descent: Step Size

- $J(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 5)^2 + (\mathbf{x}_2 10)^2$
- Which step size to take?
- Controlled by parameter α
 - called learning rate
- From previous example:
 - a = [10 5]
 - $-\nabla J(a) = [-10 \ 10]$
- Let $\alpha = 0.2$
- $\mathbf{a} \alpha \nabla \mathbf{J}(\mathbf{a}) = [10 \ 5] + 0.2 [-10 \ 10] = [8 \ 7]$
- J(10, 5) = 50; J(8,7) = 18



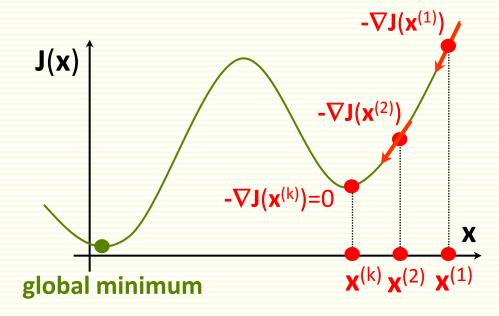
Gradient Descent Algorithm

$$\mathbf{k} = 1$$
 $\mathbf{x}^{(1)} = \text{any initial guess}$
 $\text{choose } \alpha, \varepsilon$
 $\text{while } \alpha || \nabla \mathbf{J}(\mathbf{x}^{(k)}) || > \varepsilon$
 $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha \nabla \mathbf{J}(\mathbf{x}^{(k)})$
 $\mathbf{k} = \mathbf{k} + 1$



Gradient Descent: Local Minimum

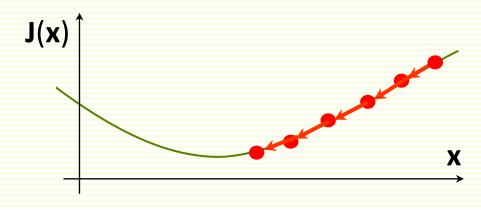
- Not guaranteed to find global minimum
 - gets stuck in local minimum



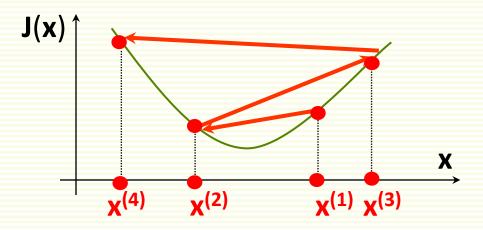
 Still gradient descent is very popular because it is simple and applicable to any differentiable function

How to Set Learning Rate α ?

 If α too small, too many iterations to converge



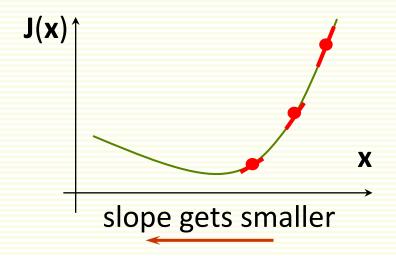
 If α too large, may overshoot the local minimum and possibly never even converge



 It helps to compute J(x) as a function of iteration number, to make sure we are properly minimizing it

How to Set Learning Rate α ?

- As we approach local minimum, often gradient gets smaller
- Step size may get smaller automatically, even if α is fixed
- So it may be unnecessary to decrease α over time in order not to overshoot a local minimum



Variable Learning Rate

• If desired, can change learning rate α at each iteration

$$\mathbf{k} = 1$$
 $\mathbf{x}^{(1)} = \text{any initial guess}$
 $\text{choose } \alpha, \epsilon$
 $\text{while } \alpha || \nabla J(\mathbf{x}^{(k)}) || > \epsilon$
 $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha \nabla J(\mathbf{x}^{(k)})$
 $\mathbf{k} = \mathbf{k} + 1$

$$\mathbf{k} = 1$$
 $\mathbf{x}^{(1)} = \text{any initial guess}$
 $\text{choose } \mathbf{\epsilon}$
 $\text{while } \alpha || \nabla \mathbf{J}(\mathbf{x}^{(k)}) || > \mathbf{\epsilon}$
 $\text{choose } \alpha^{(k)}$
 $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha^{(k)} \nabla \mathbf{J}(\mathbf{x}^{(k)})$
 $\mathbf{k} = \mathbf{k} + 1$

Variable Learning Rate

Usually don't keep track of all intermediate solutions

$$\begin{aligned} &\textbf{k} = 1 \\ &\textbf{x}^{(1)} = \text{any initial guess} \\ &\text{choose } \alpha, \epsilon \\ &\textbf{while } \alpha ||\nabla J(\textbf{x}^{(k)})|| > \epsilon \\ &\textbf{x}^{(k+1)} = \textbf{x}^{(k)} - \alpha \, \nabla J(\textbf{x}^{(k)}) \\ &\textbf{k} = \textbf{k} + 1 \end{aligned} \qquad \qquad \begin{aligned} &\textbf{x} = \text{any initial guess} \\ &\text{choose } \alpha, \epsilon \\ &\textbf{while } \alpha ||\nabla J(\textbf{x})|| > \epsilon \\ &\textbf{x} = \textbf{x} - \alpha \, \nabla J(\textbf{x}) \end{aligned}$$

Advanced Optimization Methods

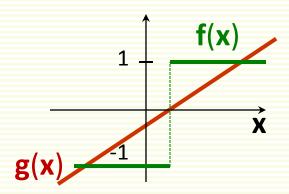
- There are more advanced gradient-based optimization methods
- Such as conjugate gradient
 - ullet automatically pick a good learning rate α
 - usually converge faster
 - however more complex to understand and implement
 - in Matlab, use fminunc for various advanced optimization methods

Supervised Machine Learning (Recap)

- Chose a learning machine f(x,w)
 - w are tunable weights, x is the input example
 - f(x,w) should output the correct class of sample x
 - use labeled samples to tune weights w so that f(x,w) give the correct class (correct y) for example x
- How to choose a learning machine f(x,w)?
 - many choices possible
 - previous lecture: kNN classifier
 - this lecture: linear classifier

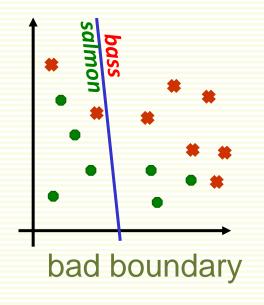
Linear Classifier: 2 Classes

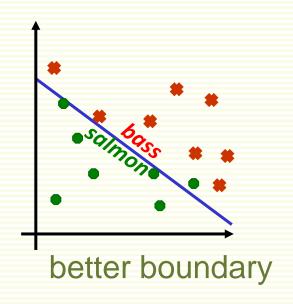
- First consider the two-class case
- We choose the following encoding:
 - y = 1 for the first class
 - y = -1 for the second class



- Linear classifier
 - linear function: $-\infty \le \mathbf{w}_0 + \mathbf{x}_1 \mathbf{w}_1 + ... + \mathbf{x}_d \mathbf{w}_d \le \infty$
 - we need f(x,w) to be either +1 or -1
 - let $g(x,w) = w_0 + x_1 w_1 + ... + x_d w_d$
 - let f(x,w) = sign(g(x,w))
 - 1 if g(x,w) is positive
 - -1 if **g(x,w)** is negative
 - g(x,w) is called the discriminant function

Linear Classifier: Decision Boundary

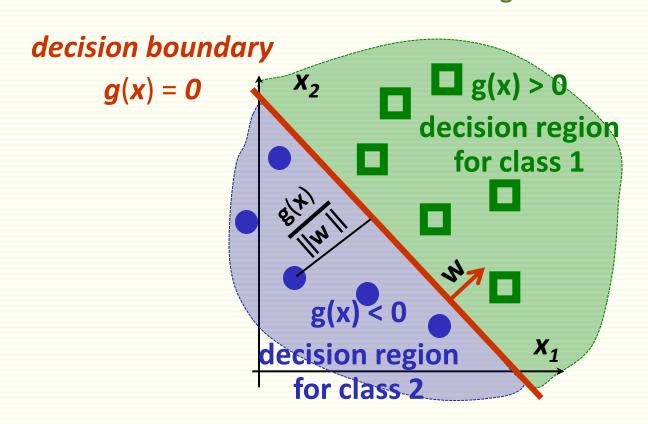




- $f(x,w) = sign(g(x,w)) = sign(w_0+x_1w_1+...+x_dw_d)$
- Decision boundary is linear
- Find the best linear boundary to separate two classes
 - Search for best $\mathbf{w} = [\mathbf{w}_0, \mathbf{w}_1, ..., \mathbf{w}_d]$ to minimize training error

More on Linear Discriminant Function (LDF)

- LDF: $g(x,w) = w_0 + x_1 w_1 + ... + x_d w_d$
- Written using vector notation $g(x) = w^t x + w_0$ weight vector bias or threshold



More on Linear Discriminant Function (LDF)

- Decision boundary: $\mathbf{g}(\mathbf{x},\mathbf{w}) = \mathbf{w}_0 + \mathbf{x}_1 \mathbf{w}_1 + \dots + \mathbf{x}_d \mathbf{w}_d = 0$
- This is a hyperplane, by definition
 - a point in 1D
 - a line in 2D
 - a plane in 3D
 - a hyperplane in higher dimensions

Multiple Classes

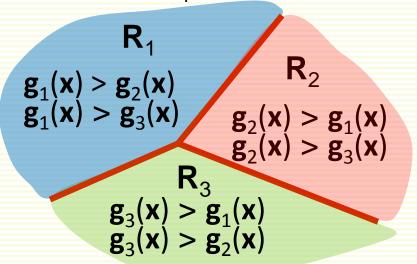
- We have m classes
- Define m linear discriminant functions

$$\mathbf{g}_{i}(\mathbf{x}) = \mathbf{w}_{i}^{t}\mathbf{x} + \mathbf{w}_{i0}$$
 for $\mathbf{i} = 1, 2, ... \mathbf{m}$

Assign x to class i if

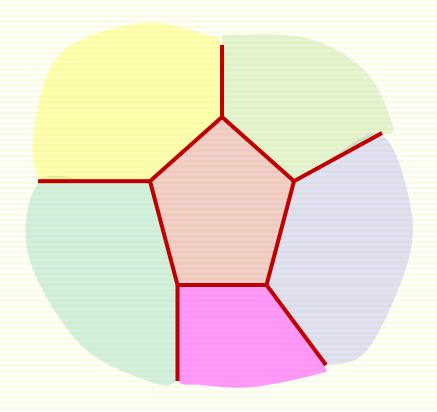
$$g_i(x) > g_i(x)$$
 for all $j \neq i$

- Let R_i be the decision region for class i
 - That is all examples in R_i get assigned class i



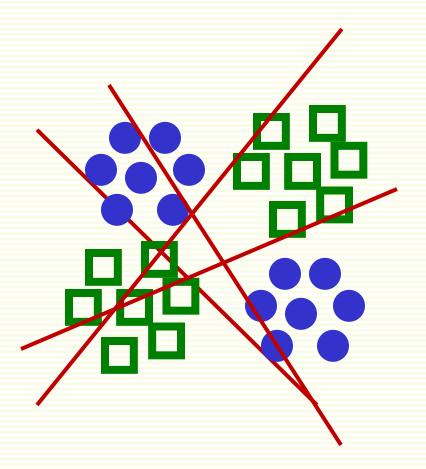
Multiple Classes

- Can be shown that decision regions are convex
- In particular, they must be spatially contiguous



Failure Cases for Linear Classifier

- Thus applicability of linear classifiers is limited to mostly unimodal distributions, such as Gaussian
- Not unimodal data
- Need non-contiguous decision regions
- Linear classifier will fail



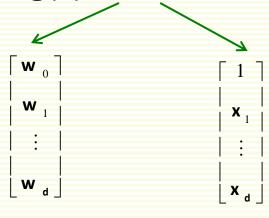
Fitting Parameters w

Linear discriminant function g(x) = w^tx + w₀

• Can rewrite it
$$\mathbf{g}(\mathbf{x}) = \begin{bmatrix} \mathbf{w}_0 & \mathbf{w}^t \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ \mathbf{x} \end{bmatrix} = \mathbf{a}^t \mathbf{z} = \mathbf{g}(\mathbf{z})$$

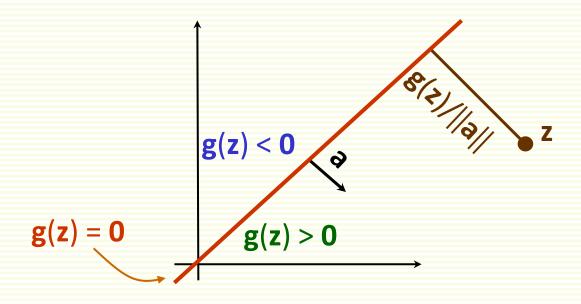
new weight vector \mathbf{a} new feature vector \mathbf{z}

- z is called augmented feature vector
- new problem equivalent to the old g(z) = a^tz



Augmented Feature Vector

- Feature augmenting is done to simplify notation
- From now on we assume that we have augmented feature vectors
 - given samples x¹,..., xⁿ convert them to augmented samples z¹,..., zⁿ by adding a new dimension of value 1
- $g(z) = a^t z$



Training Error

- For the rest of the lecture, assume we have 2 classes
- Samples z¹,..., zⁿ some in class 1, some in class 2
- Use these samples to determine weights a in the discriminant function g(z) = a^tz
- Want to minimize number of misclassified samples

• Recall that
$$\begin{cases} \mathbf{g}(\mathbf{z}^{i}) > 0 \implies \text{class 1} \\ \mathbf{g}(\mathbf{z}^{i}) < 0 \implies \text{class 2} \end{cases}$$

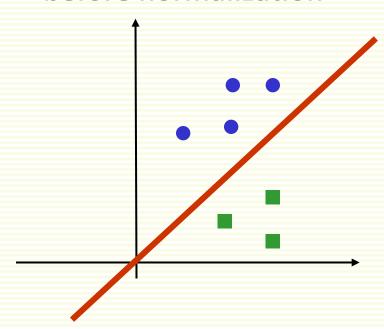
• Thus training error is 0 if $\begin{cases} \mathbf{g}(\mathbf{z}^i) > 0 & \forall \mathbf{z}^i \text{ class 1} \\ \mathbf{g}(\mathbf{z}^i) < 0 & \forall \mathbf{z}^i \text{ class 2} \end{cases}$

Simplifying Notation Further

- Thus training error is 0 if $\begin{cases} \mathbf{a^t z^i} > 0 & \forall \mathbf{z^i} \text{ class 1} \\ \mathbf{a^t z^i} < 0 & \forall \mathbf{z^i} \text{ class 2} \end{cases}$
- Equivalently, training error is 0 if $\begin{cases} \mathbf{a^t z^i} > 0 \ \forall \mathbf{z^i} \text{ class 1} \\ \mathbf{a^t (-z^i)} > 0 \ \forall \mathbf{z^i} \text{ class 2} \end{cases}$
- Problem "normalization":
 - 1. replace all examples zⁱ from class 2 by -zⁱ
 - 2. seek weights **a** s.t. $\mathbf{a}^{t}\mathbf{z}^{i} > 0$ for $\forall \mathbf{z}^{i}$
- If exists, such **a** is called a **separating** or **solution** vector
- Original samples x¹,... xⁿ can also be linearly separated

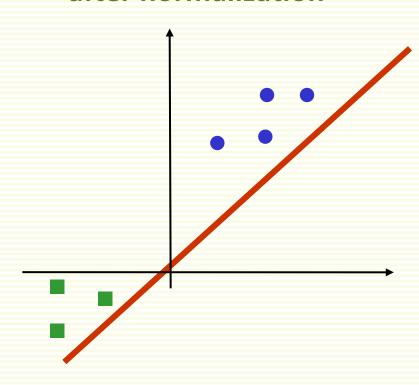
Effect of Normalization

before normalization



seek a hyperplane that separates samples from different categories

after normalization

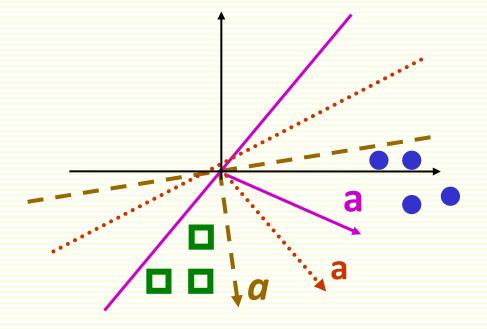


seek hyperplane that puts normalized samples on the same (positive) side

Solution Region

• Find weight vector **a** s.t. for all samples **z**¹,...,**z**ⁿ

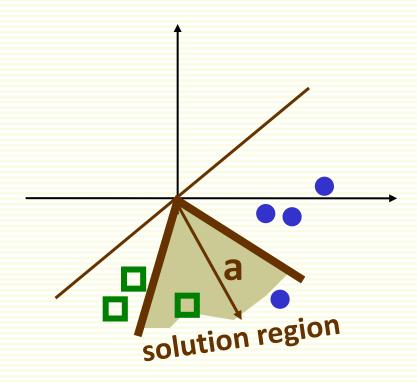
$$a^{t}z^{i} = \sum_{k=0}^{d} a_{k}z_{d}^{i} > 0$$



If there is one such a, then there are infinitely many a

Solution Region

• Solution region: the set of all possible solutions for a



Criterion Function: First Attempt

- Find weight vector **a** s.t. $\forall z^1,..., z^n$, $a^t z^i > 0$
- Design a criterion function J(a), which is minimum when a is a solution vector
- Let Z(a) be the set of examples misclassified by a

$$Z(a) = \{ z^i \mid a^t z^i < 0 \}$$

Natural choice: number of misclassified examples

$$J(a) = |Z(a)|$$

- Unfortunately, can't be minimized with gradient descent
 - piecewise constant, gradient zero or does not exist

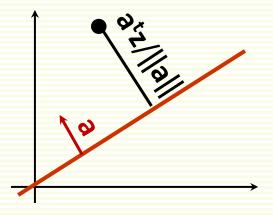


Perceptron Criterion Function

• Better choice: Perceptron criterion function

$$J_{p}(a) = \sum_{z \in Z(a)} (-a^{t}z)$$

- If z is misclassified, a^tz < 0
- Thus $J(a) \ge 0$
- J_p(a) is proportional to the sum of distances of misclassified examples to decision boundary
- J_p(a) is piecewise linear and suitable for gradient descent





Optimizing with Gradient Descent

$$J_{p}(a) = \sum_{z \in Z(a)} (-a^{t}z)$$

- Gradient of $J_p(a)$ is $\nabla J_p(a) = \sum_{z \in Z(a)} (-z)$
 - cannot solve $\nabla \mathbf{J}_{p}(\mathbf{a}) = 0$ analytically because of $\mathbf{Z}(\mathbf{a})$
- Recall update rule for gradient descent

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k+1)} - \alpha \nabla \mathbf{J}(\mathbf{x}^{(k)})$$

Gradient decent update rule for J_p(a) is:

$$\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \alpha \sum_{\mathbf{z} \in \mathbf{Z}(\mathbf{a})} \mathbf{z}$$

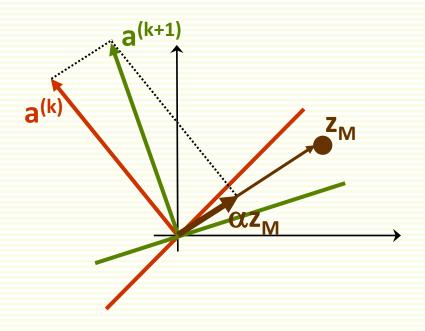
- called batch rule because it is based on all examples
- true gradient descent

Perceptron Single Sample Rule

• Gradient decent single sample rule for $J_p(a)$ is

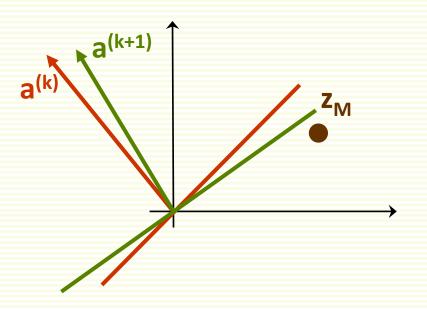
$$\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \alpha \cdot \mathbf{z}_{\mathbf{M}}$$

- **z**_M is one sample misclassified by **a**^(k)
- must have a consistent way to visit samples
- Geometric Interpretation:
- z_M misclassified by $a^{(k)}$ $(a^{(k)})^t z_M \le 0$
- z_M is on the wrong side of decision boundary
- adding $\alpha \cdot \mathbf{z_M}$ to a moves decision boundary in the right direction

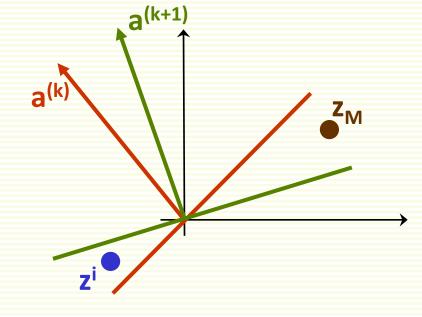


Perceptron Single Sample Rule

if α is too small, \mathbf{z}_{M} is still misclassified



if α is too large, previously correctly classified sample \mathbf{z}^i is now misclassified



Perceptron Single Sample Rule Example

	features				grade
name	good attendance?	tall?	sleeps in class?	chews gum?	
Jane	yes (1)	yes (1)	no (-1)	no (-1)	А
Steve	yes (1)	yes (1)	yes (1)	yes (1)	F
Mary	no (-1)	no (-1)	no (-1)	yes (1)	F
Peter	yes (1)	no (-1)	no (-1)	yes (1)	Α

- class 1: students who get grade A
- class 2: students who get grade F

Augment Feature Vector

	features			grade		
name	extra	good attendance?	tall?	sleeps in class?	chews gum?	
Jane	1	yes (1)	yes (1)	no (-1)	no (-1)	Α
Steve	1	yes (1)	yes (1)	yes (1)	yes (1)	F
Mary	1	no (-1)	no (-1)	no (-1)	yes (1)	F
Peter	1	yes (1)	no (-1)	no (-1)	yes (1)	Α

convert samples x¹,..., xⁿ to augmented samples z¹,..., zⁿ
 by adding a new dimension of value 1

"Normalization"

	features			grade		
name	extra	good attendance?	tall?	sleeps in class?	chews gum?	
Jane	1	yes (1)	yes (1)	no (-1)	no (-1)	Α
Steve	-1	yes (-1)	yes (-1)	yes (-1)	yes (-1)	F
Mary	-1	no (1)	no (1)	no (1)	yes (-1)	F
Peter	1	yes (1)	no (-1)	no (-1)	yes (1)	Α

Replace all examples from class 2 by their negative

$$z^i \rightarrow - z^i$$

Seek weight vector a s.t. a^tzⁱ > 0 for all zⁱ

	features			grade		
name	extra	good attendance?	tall?	sleeps in class?	chews gum?	
Jane	1	yes (1)	yes (1)	no (-1)	no (-1)	А
Steve	-1	yes (-1)	yes (-1)	yes (-1)	yes (-1)	F
Mary	-1	no (1)	no (1)	no (1)	yes (-1)	F
Peter	1	yes (1)	no (-1)	no (-1)	yes (1)	Α

- Gradient descent single sample rule: $\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \alpha \cdot \mathbf{z}_{\mathbf{M}}$
- Set fixed learning rate to $\alpha = 1$: $\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \mathbf{z}_{\mathbf{M}}$
- Sample is misclassified if $a^t z^i = \sum_{k=0}^{\infty} a_k z_k^i < 0$

- initial weights a⁽¹⁾ = [0.25, 0.25, 0.25, 0.25]
- visit all samples sequentially

name	a ^t z	misclassified?
Jane	0.25*1+0.25*1+0.25*1+0.25*(-1)+0.25*(-1) >0	no
Steve	0.25*(-1)+0.25*(-1)+0.25*(-1)+0.25*(-1)+0.25*(-1)<0	yes

new weights

$$\mathbf{a}^{(2)} = \mathbf{a}^{(1)} + \mathbf{z}_{\mathbf{M}} = \begin{bmatrix} 0.25 & 0.25 & 0.25 & 0.25 \end{bmatrix} +$$

$$+ \begin{bmatrix} -1 & -1 & -1 & -1 & -1 \end{bmatrix} =$$

$$= \begin{bmatrix} -0.75 & -0.75 & -0.75 & -0.75 & -0.75 \end{bmatrix}$$

$$\mathbf{a}^{(2)} = \begin{bmatrix} -0.75 & -0.75 & -0.75 & -0.75 \end{bmatrix}$$

name	a^tz	misclassified?
Mary	-0.75*(-1)-0.75*1 -0.75 *1 -0.75 *1 -0.75*(-1) <0	yes

new weights

$$\mathbf{a}^{(3)} = \mathbf{a}^{(2)} + \mathbf{z}_{M} = \begin{bmatrix} -0.75 & -0.75 & -0.75 & -0.75 \end{bmatrix} +$$

$$+ \begin{bmatrix} -1 & 1 & 1 & 1 & -1 \end{bmatrix} =$$

$$= \begin{bmatrix} -1.75 & 0.25 & 0.25 & 0.25 & -1.75 \end{bmatrix}$$

$$a^{(3)} = \begin{bmatrix} -1.75 & 0.25 & 0.25 & 0.25 & -1.75 \end{bmatrix}$$

name	a ^t z	misclassified?
Peter	-1.75 *1 +0.25 * 1+0.25 * (-1) +0.25 * (-1)-1.75 *1 <0	yes

new weights

$$\mathbf{a}^{(4)} = \mathbf{a}^{(3)} + \mathbf{z}_{M} = \begin{bmatrix} -1.75 & 0.25 & 0.25 & 0.25 & -1.75 \end{bmatrix} +$$

$$+ \begin{bmatrix} 1 & 1 & -1 & -1 & 1 \end{bmatrix} =$$

$$= \begin{bmatrix} -0.75 & 1.25 & -0.75 & -0.75 & -0.75 \end{bmatrix}$$

Single Sample Rule: Convergence

$$\mathbf{a}^{(4)} = \begin{bmatrix} -0.75 & 1.25 & -0.75 & -0.75 \end{bmatrix}$$

name	a ^t z	misclassified?
Jane	-0.75 *1 +1.25*1 -0.75*1 -0.75 *(-1) -0.75 *(-1)+0	no
Steve	-0.75*(-1)+1.25*(-1) -0.75*(-1) -0.75*(-1)-0.75*(-1)>0	no
Mary	-0.75 *(-1)+1.25*1-0.75*1 -0.75 *1 -0.75*(-1) >0	no
Peter	-0.75 *1+ 1.25*1-0.75* (-1)-0.75* (-1) -0.75 *1 >0	no

Thus the discriminant function is

$$\mathbf{g}(\mathbf{z}) = -0.75 \ \mathbf{z}_0 + 1.25 \mathbf{z}_1 - 0.75 \mathbf{z}_2 - 0.75 \mathbf{z}_3 - 0.75 \mathbf{z}_4$$

Converting back to the original features x

$$\mathbf{g}(\mathbf{x}) = 1.25\mathbf{x}_1 - 0.75\mathbf{x}_2 - 0.75\mathbf{x}_3 - 0.75\mathbf{x}_4 - 0.75$$

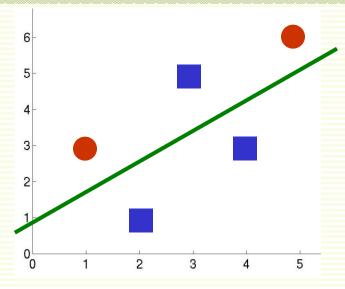
Final Classifier

- Trained LDF: $\mathbf{g}(\mathbf{x}) = 1.25x_1 0.75x_2 0.75x_3 0.75x_4 0.75$
- Leads to classifier:

$$1.25x_1 - 0.75x_2 - 0.75x_3 - 0.75x_4 > 0.75 \Rightarrow \text{grade A}$$
good tall sleeps in class chews gum
attendance

- This is just one possible solution vector
- With $\mathbf{a}^{(1)}=[0,0.5,0.5,0.5,0]$, solution is [-1,1.5,-0.5,-1,-1] $1.5\mathbf{x}_1 - 0.5\mathbf{x}_2 - \mathbf{x}_3 - \mathbf{x}_4 > 1 \Rightarrow \text{grade } \mathbf{A}$
 - In this solution, being tall is the least important feature

- Suppose we have examples:
 - class 1: [2,1], [4,3], [3,5]
 - class 2: [1,3], [5,6]
 - not linearly separable
- Still would like to get approximate separation

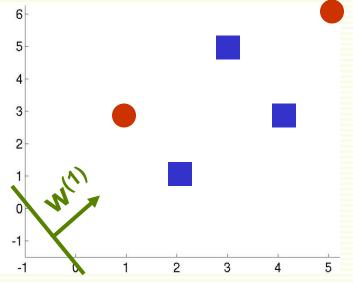


- Good line choice is shown in green
- Let us run gradient descent
 - Add extra feature and "normalize"

$$\mathbf{z}^{1} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \qquad \mathbf{z}^{2} = \begin{bmatrix} 4 \\ 3 \end{bmatrix} \qquad \mathbf{z}^{3} = \begin{bmatrix} 3 \\ 4 \end{bmatrix} \qquad \mathbf{z}^{4} = \begin{bmatrix} -1 \\ -1 \end{bmatrix} \qquad \mathbf{z}^{5} = \begin{bmatrix} -1 \\ -5 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ 3 \end{bmatrix} \qquad \begin{bmatrix} 5 \end{bmatrix} \qquad \begin{bmatrix}$$

- single sample perceptron rule
- Initial weights a⁽¹⁾ = [1 1 1]
- This is line $x_1 + x_2 + 1 = 0$
- Use fixed learning rate $\alpha = 1$
- Rule is: $a^{(k+1)} = a^{(k)} + z_M$

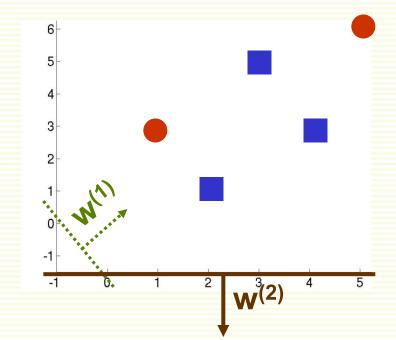


$$\mathbf{z}^{1} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \quad \mathbf{z}^{2} = \begin{bmatrix} 4 \\ 3 \end{bmatrix} \quad \mathbf{z}^{3} = \begin{bmatrix} 3 \\ 4 \end{bmatrix} \quad \mathbf{z}^{4} = \begin{bmatrix} -1 \\ -1 \end{bmatrix} \quad \mathbf{z}^{5} = \begin{bmatrix} -5 \\ -6 \end{bmatrix}$$

- $\mathbf{a}^{t}\mathbf{z}^{1} = [1 \ 1 \ 1] \cdot [1 \ 2 \ 1]^{t} > 0$
- $\mathbf{a}^{t}\mathbf{z}^{2} = [1 \ 1 \ 1] \cdot [1 \ 4 \ 3]^{t} > 0$
- $\mathbf{a}^{t}\mathbf{z}^{3} = [1 \ 1 \ 1] \cdot [1 \ 3 \ 5]^{t} > 0$

- $a^{(1)} = [1 \ 1 \ 1]$
- rule is: $a^{(k+1)} = a^{(k)} + z_M$

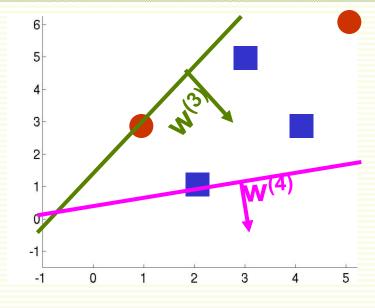
$$\mathbf{z}^{1} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} \quad \mathbf{z}^{2} = \begin{bmatrix} 1 \\ 4 \\ 1 \end{bmatrix} \quad \mathbf{z}^{3} = \begin{bmatrix} 1 \\ 3 \\ 1 \end{bmatrix} \quad \mathbf{z}^{4} = \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} \quad \mathbf{z}^{5} = \begin{bmatrix} -1 \\ -5 \\ -6 \end{bmatrix}$$



- $\mathbf{a}^{t}\mathbf{z}^{4} = [1 \ 1 \ 1] \cdot [-1 \ -1 \ -3]^{t} = -5 < 0$
- Update: $\mathbf{a}^{(2)} = \mathbf{a}^{(1)} + \mathbf{z}_{M} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} -1 & -1 & -3 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -2 \end{bmatrix}$
- $\mathbf{a}^{t}\mathbf{z}^{5} = [0\ 0\ -2] \cdot [-1\ -5\ -6]^{t} = 12 > 0$
- $\mathbf{a}^{t}\mathbf{z}^{1} = [0 \ 0 \ -2] \cdot [1 \ 2 \ 1]^{t} < 0$
- Update: $\mathbf{a}^{(3)} = \mathbf{a}^{(2)} + \mathbf{z}_{M} = [0 \ 0 \ -2] + [1 \ 2 \ 1] = [1 \ 2 \ -1]$

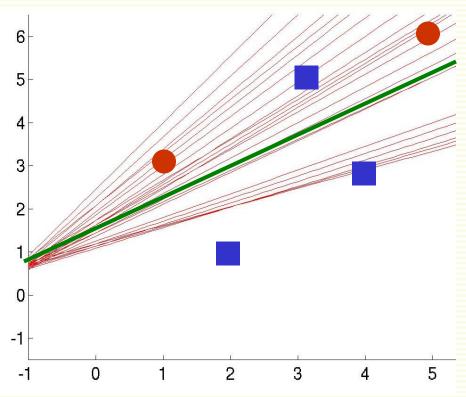
- $a^{(3)} = [1 \ 2 \ -1]$
- rule is: $a^{(k+1)} = a^{(k)} + z_M$

$$\mathbf{z}^{1} = \begin{bmatrix} \mathbf{1} \\ \mathbf{2} \\ \mathbf{z}^{2} \end{bmatrix} \quad \mathbf{z}^{2} = \begin{bmatrix} \mathbf{4} \\ \mathbf{3} \end{bmatrix} \quad \mathbf{z}^{3} = \begin{bmatrix} \mathbf{3} \\ \mathbf{3} \\ \mathbf{z}^{4} \end{bmatrix} \quad \mathbf{z}^{4} = \begin{bmatrix} -1 \\ -1 \\ \mathbf{z}^{5} \end{bmatrix} \quad \mathbf{z}^{5} = \begin{bmatrix} -5 \\ -6 \end{bmatrix}$$



- $\mathbf{a}^{t}\mathbf{z}^{2} = [1 \ 4 \ 3] \cdot [1 \ 2 \ -1]^{t} = 6 > 0$
- $\mathbf{a}^{t}\mathbf{z}^{3} = [1 \ 3 \ 5] \cdot [1 \ 2 \ -1]^{t} = 2 > 0$
- $\mathbf{a}^{t}\mathbf{z}^{4} = [-1 \ -1 \ -3] \cdot [1 \ 2 \ -1]^{t} = 0$
- Update: $\mathbf{a}^{(4)} = \mathbf{a}^{(3)} + \mathbf{z}_{M} = \begin{bmatrix} 1 & 2 & -1 \end{bmatrix} + \begin{bmatrix} -1 & -1 & -3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & -4 \end{bmatrix}$

- We can continue this forever
 - there is no solution vector a satisfying for all a^tz_i > 0 for all i
- Need to stop at a good point
- Solutions at iterations
 900 through 915
- Some are good some are not
- How do we stop at a good solution?



Convergence of Perceptron Rules

1. Classes are linearly separable:

- with fixed learning rate, both single sample and batch rules converge to a correct solution a
- can be any a in the solution space

2. Classes are not linearly separable:

- with fixed learning rate, both single sample and batch do not converge
- can ensure convergence with appropriate variable learning rate
 - $\alpha \rightarrow 0$ as $k \rightarrow \infty$
 - example, inverse linear: $\alpha = c/k$, where c is any constant
 - also converges in the linearly separable case
 - no guarantee that we stop at a good point, but there are good reasons to choose inverse linear learning rate
- Practical Issue: both single sample and batch algorithms converge faster if features are roughly on the same scale
 - see kNN lecture on feature normalization

Batch vs. Single Sample Rules

Batch

- True gradient descent, full gradient computed
- Smoother gradient because all samples are used
- Takes longer to converge

Single Sample

- Only partial gradient is computed
- Noisier gradient, therefore may concentrates more than necessary on any isolated training examples (those could be noise)
- Converges faster
- Easier to analyze

Minimum Squared Error Optimization

Idea: convert to easier and better understood problem

a^tzⁱ > 0 for all samples zⁱsolve system of linear inequalities

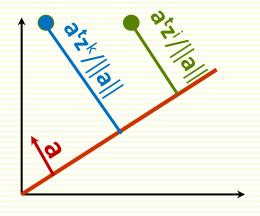
 $\mathbf{a}^{t}\mathbf{z}^{i} = \mathbf{b}_{i}$ for all samples \mathbf{z}^{i} solve system of linear equations

- MSE procedure
 - choose positive constants b₁, b₂,..., b_n
 - try to find weight vector a s.t. a^tzⁱ = b_i for all samples zⁱ
 - if succeed, then **a** is a solution because **b**_i's are positive
 - consider all the samples (not just the misclassified ones)

MSE: Margins

- By setting a^tzⁱ = b_i, we expect zⁱ to be at a relative distance b_i from the separating hyperplane
- Thus b₁, b₂,..., b_n are expected relative distances of examples from the separating 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 such information, there are good reasons to set

$$\mathbf{b}_1 = \mathbf{b}_2 = \dots = \mathbf{b}_n = 1$$



MSE: Matrix Notation

• Solve system of **n** equations $\begin{cases} a^{t}z^{1} = b_{1} \\ \vdots \\ a^{t}z^{n} = b_{n} \end{cases}$

$$\begin{cases} \vdots \\ \mathbf{a}^{t} \mathbf{z}^{n} = \mathbf{b}_{n} \end{cases}$$

• Using matrix notation:

$$\begin{bmatrix} \mathbf{z}_{0}^{1} & \mathbf{z}_{1}^{1} & \cdots & \mathbf{z}_{d}^{1} \\ \mathbf{z}_{0}^{2} & \mathbf{z}_{1}^{2} & \cdots & \mathbf{z}_{d}^{2} \end{bmatrix} \begin{bmatrix} \mathbf{a}_{0} \\ \mathbf{a}_{1} \\ \vdots \\ \vdots \\ \mathbf{z}_{0}^{n} & \mathbf{z}_{1}^{n} & \cdots & \mathbf{z}_{d}^{n} \end{bmatrix} \begin{bmatrix} \mathbf{a}_{0} \\ \mathbf{a}_{1} \\ \vdots \\ \vdots \\ \vdots \\ \mathbf{a}_{d} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{1} \\ \mathbf{b}_{2} \\ \vdots \\ \vdots \\ \vdots \\ \mathbf{b}_{n} \end{bmatrix}$$

$$\mathbf{Z}$$

Solve a linear system Za = b

MSE: Exact Solution is Rare

- Solve a linear system Za = b
 - **Z** is an **n** by (**d** +**1**) matrix
- Exact solution can be found only if Z is nonsingular and square, in which case inverse Z⁻¹ exists
 - $a = Z^{-1}b$
 - (number of samples) = (number of features + 1)
 - if happens, guaranteed to find separating hyperplane
 - but almost never happens in practice

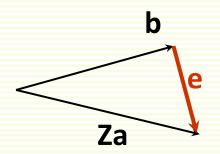
MSE:Approximate Solution

- Typically Z is overdetermined
 - more rows (examples) than columns (features)

- No exact solution for Za = b in this case
- Find an approximate solution a, that is Za ≈ b
 - approximate solution a does not necessarily give a separating hyperplane in the separable case
 - but hyperplane corresponding to an approximate a may still be a good solution

MSE Criterion Function

 MSE approach: find a which minimizes the length of the error vector e = Za - b



Minimize the minimum squared error criterion function:

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

Can be optimized exactly

MSE: Optimizing $J_s(a)$

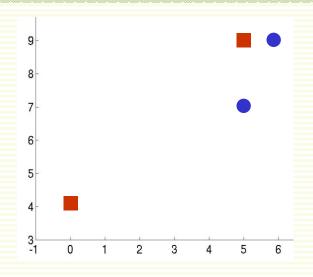
$$J_{s}(a) = \|Za - b\|^{2} = \sum_{i=1}^{n} (a^{t}z^{i} - b_{i})^{2}$$

- Compute the gradient: $\nabla J_s(a) = 2Z^t(Za-b)$
- Set it to zero: 2**Z**^t(**Za-b**) = 0
- If Z^tZ is non-singular, its inverse exists and can find a unique solution for a = (Z^tZ)⁻¹ Z^tb
- In Matlab
 - a = Z\b
 - or use pinv command (pseudo-inverse)
 - a = pinv(Z)*b;

MSE: Example

- Class 1: (6 9), (5 7)
- Class 2: (5 9), (0 4)
- Add extra feature and "normalize"

$$\mathbf{z}^{1} = \begin{bmatrix} 1 \\ 6 \\ 9 \end{bmatrix} \quad \mathbf{z}^{2} = \begin{bmatrix} 1 \\ 5 \\ 0 \end{bmatrix} \quad \mathbf{z}^{3} = \begin{bmatrix} -1 \\ -5 \\ 0 \end{bmatrix} \quad \mathbf{z}^{4} = \begin{bmatrix} 0 \\ -4 \end{bmatrix}$$

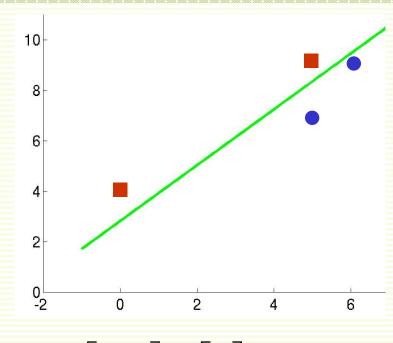


•
$$\mathbf{Z} = \begin{bmatrix} 1 & 6 & 9 \\ 1 & 5 & 7 \\ -1 & -5 & -9 \\ -1 & 0 & -4 \end{bmatrix}$$

MSE: Example

Use a=Z\b to solve in Matlab

$$\mathbf{a} = \begin{bmatrix} 2.7 \\ 1.0 \\ -0.9 \end{bmatrix}$$

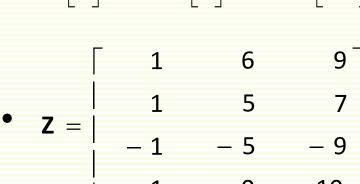


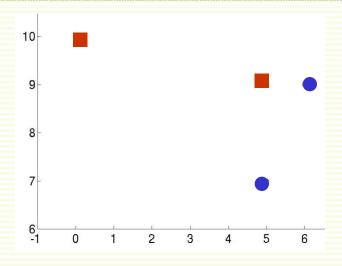
- Note **a** is an approximation since $\mathbf{Za} = \begin{bmatrix} 1.3 & | & 1 \\ 0.6 & | & | & 1 \end{bmatrix}$
- Gives a separating hyperplane since
 Za > 0

MSE: Another Example

- Class 1: (6 9), (5 7)
- Class 2: (5 9), (0 10)
- One example is far compared to others from separating hyperplane

$$\mathbf{z}^{1} = \begin{vmatrix} 6 \\ 9 \end{vmatrix} \qquad \mathbf{z}^{2} = \begin{vmatrix} 5 \\ 7 \end{vmatrix} \qquad \mathbf{z}^{3} = \begin{vmatrix} -5 \\ -9 \end{vmatrix} \qquad \mathbf{z}^{4} = \begin{vmatrix} 0 \\ -10 \end{vmatrix}$$





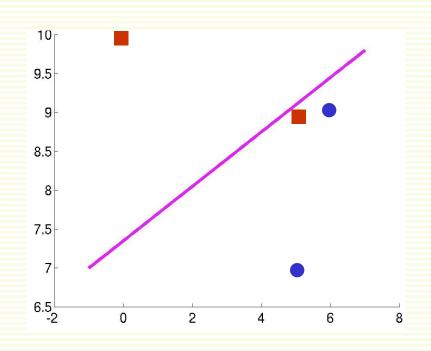
MSE: Another Example Cont.

• Choose
$$\mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

• Solve
$$\mathbf{a} = \mathbf{Z} \setminus \mathbf{b} = \begin{bmatrix} 3.2 \\ 0.2 \\ -0.4 \end{bmatrix}$$

• **Za** =
$$\begin{bmatrix} 0.2 \\ 0.9 \\ -0.04 \\ 1 \end{bmatrix}$$

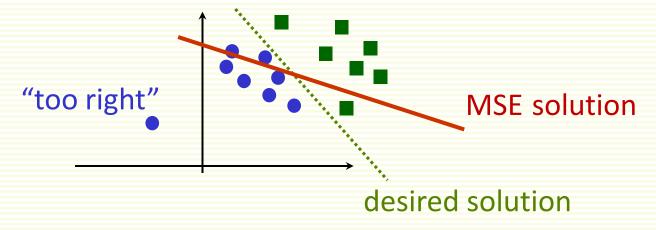
$$\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$



• Does not give a separating hyperplane since $\mathbf{a}^t \mathbf{z}^3 < \mathbf{0}$

MSE: Problems

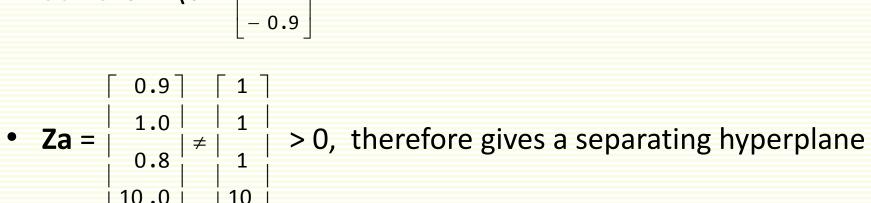
- MSE wants all examples to be at the same distance from the separating hyperplane
- Examples that are "too right", i.e. too far from the boundary cause problems

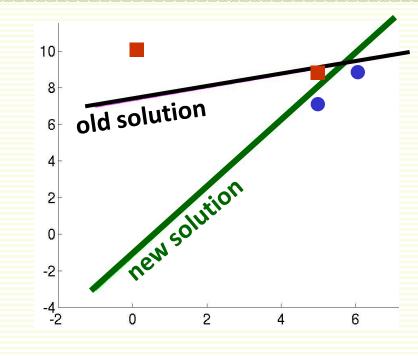


No problems with convergence though,
 both in separable and non-separable cases

MSE: Another Example Cont.

- If we know that 4th point is far from separating hyperplane
 - in practice can look at points which are furthest from the decision boundary $\begin{array}{c|c}
 & z_a = \\
 & z_a = \\$
- Set $\mathbf{b_i}$ larger for such points: $\mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$
- Solve $\mathbf{a}=\mathbf{Z}\backslash\mathbf{b}=\begin{bmatrix} -1.1\\ 1.7\\ -0.9 \end{bmatrix}$





More General Discriminant Functions

- Linear discriminant functions give simple decision boundary
 - try simpler models first
- Linear Discriminant functions are optimal for certain type of data
 - Gaussian distributions with equal covariance (don't worry if you don't know what a Gaussian is)
- May not be optimal for other data distributions, but they are very simple to use
- Discriminant functions can be more general than linear
 - For example, polynomial discriminant functions
 - Decision boundaries more complex than linear
 - Later will look more at non-linear discriminant functions

Summary

- Linear classifier works well when examples are linearly separable, or almost separable
- Two Training Approaches:
 - Perceptron Rules
 - find a separating hyperplane in the linearly separable case
 - uses gradient descent for optimization
 - 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 Rules

- converges in separable and not separable case
- can be optimized with pseudo-inverse
- but may not find separating hyperplane even if classes are linearly separable