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

$$\mathbf{J(x)} = (\mathbf{x}-5)^2$$

- 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:

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

Optimization

- How to minimize a function of many variables

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

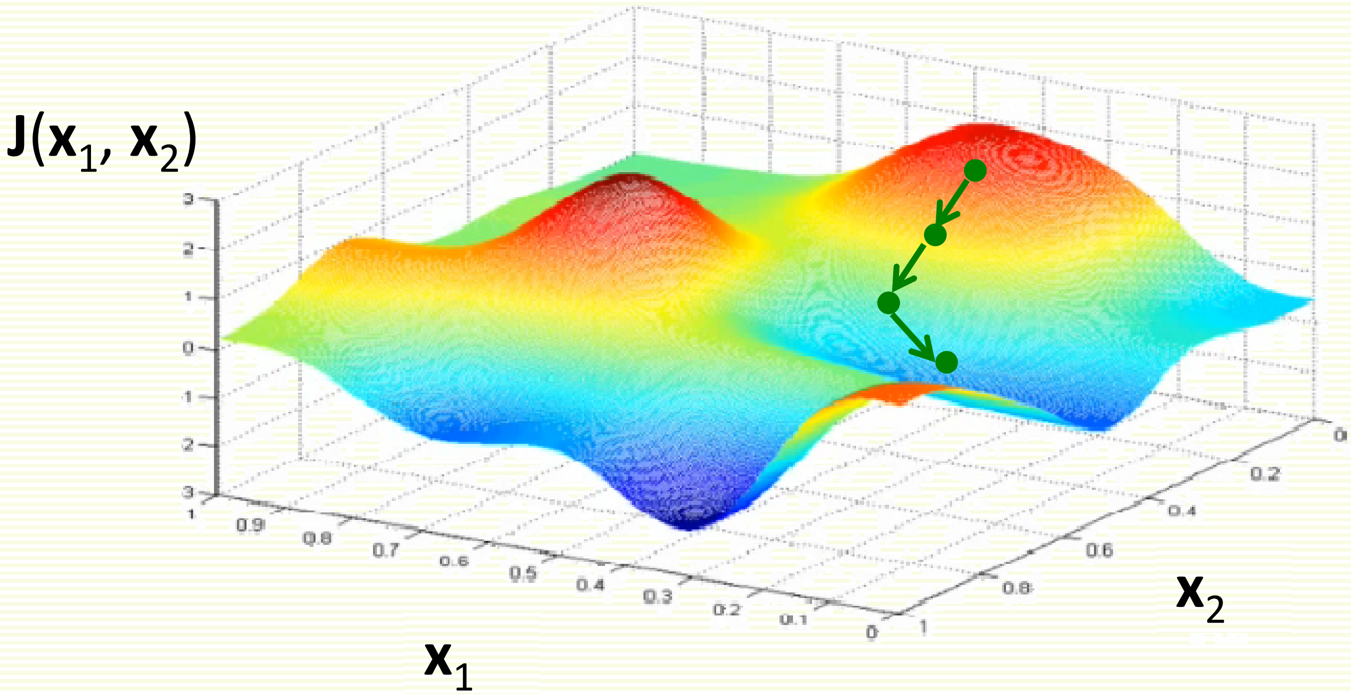
- From calculus, take partial derivatives, set them to 0

gradient

$$\begin{bmatrix} \frac{\partial}{\partial \mathbf{x}_1} \mathbf{J}(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial \mathbf{x}_d} \mathbf{J}(\mathbf{x}) \end{bmatrix} = \nabla \mathbf{J}(\mathbf{x}) = \mathbf{0}$$

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

Optimization: Gradient Direction

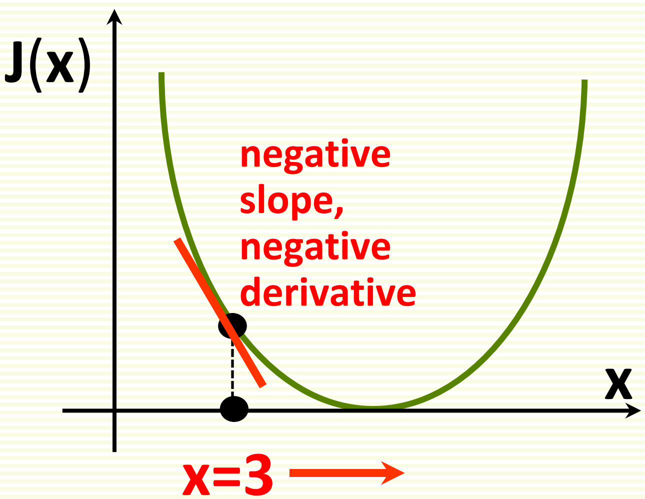


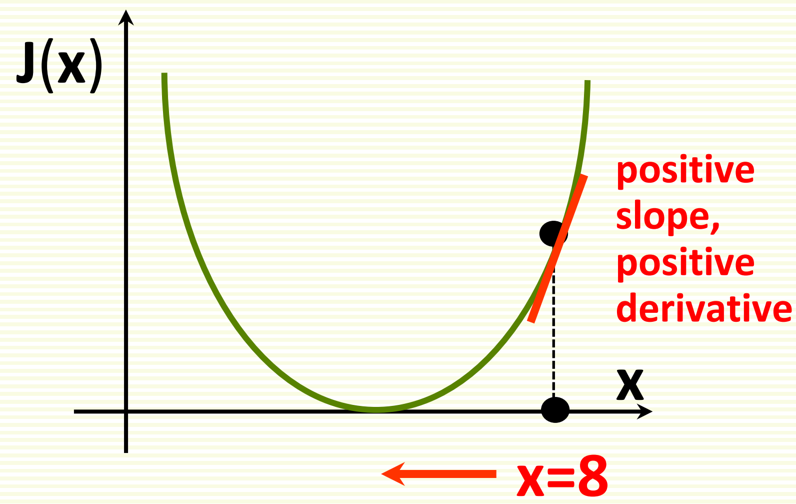
- Gradient $\nabla \mathbf{J}(\mathbf{x})$ points in the direction of steepest increase of function $\mathbf{J}(\mathbf{x})$
- **-** $\nabla \mathbf{J}(\mathbf{x})$ points in the direction of steepest decrease

Picture from Andrew Ng

Gradient Direction in 1D

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



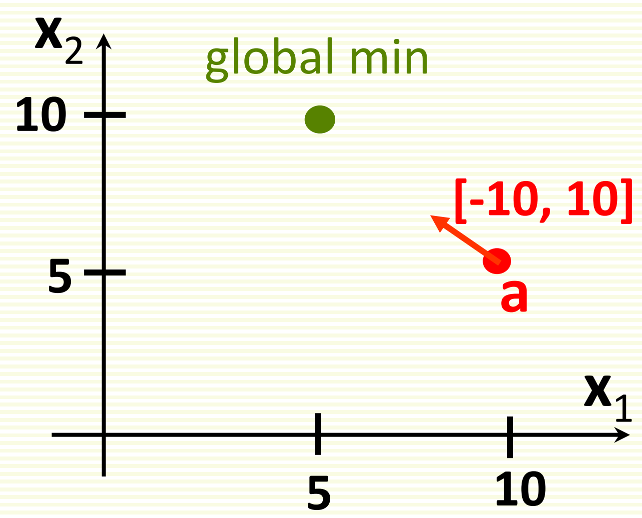


- Let $\mathbf{x} = 3$
- $-\frac{\mathbf{d}}{\mathbf{dx}}\mathbf{J}(\mathbf{3}) = \mathbf{4}$
- derivative says increase **x**

- Let $\mathbf{x} = 8$
- $-\frac{\mathbf{d}}{\mathbf{dx}}\mathbf{J}(\mathbf{3}) = -\mathbf{6}$
- derivative says decrease **x**

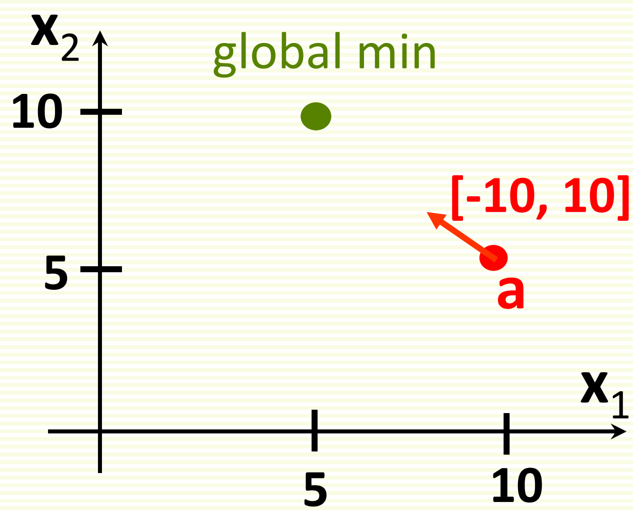
Gradient Direction in 2D

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



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:
  - $\mathbf{a} = [10 \quad 5]$
  - $-\nabla J(\mathbf{a}) = [-10 \quad 10]$
- Let $\alpha = 0.2$
- $\mathbf{a} - \alpha \nabla J(\mathbf{a}) = [10 \quad 5]+0.2\,[-10 \quad 10]=[8 \quad 7]$
- $J(10, 5) = 50$; $J(8,7) = 18$



Gradient Descent Algorithm

$\mathbf{k} = 1$

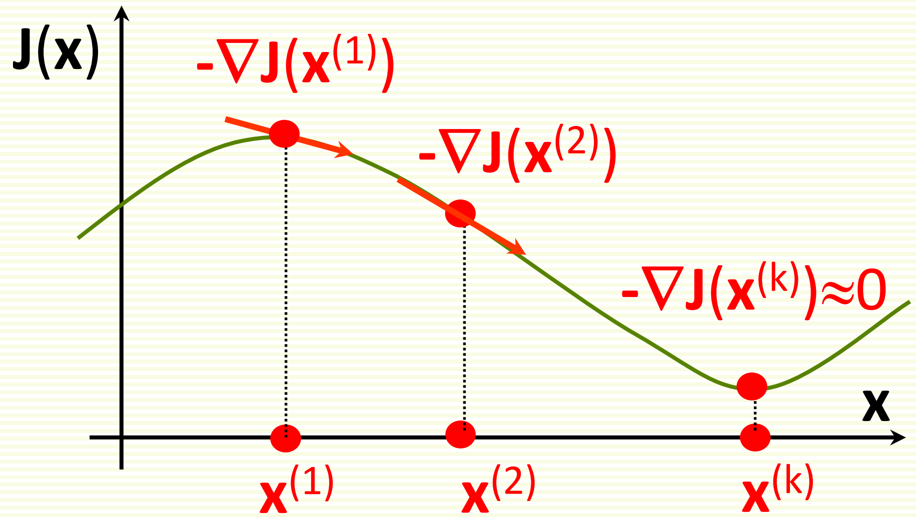
$\mathbf{x}^{(1)}$ = any initial guess

choose α, ε

while $\alpha \|\nabla \mathbf{J}(\mathbf{x}^{(k)})\| > \varepsilon$

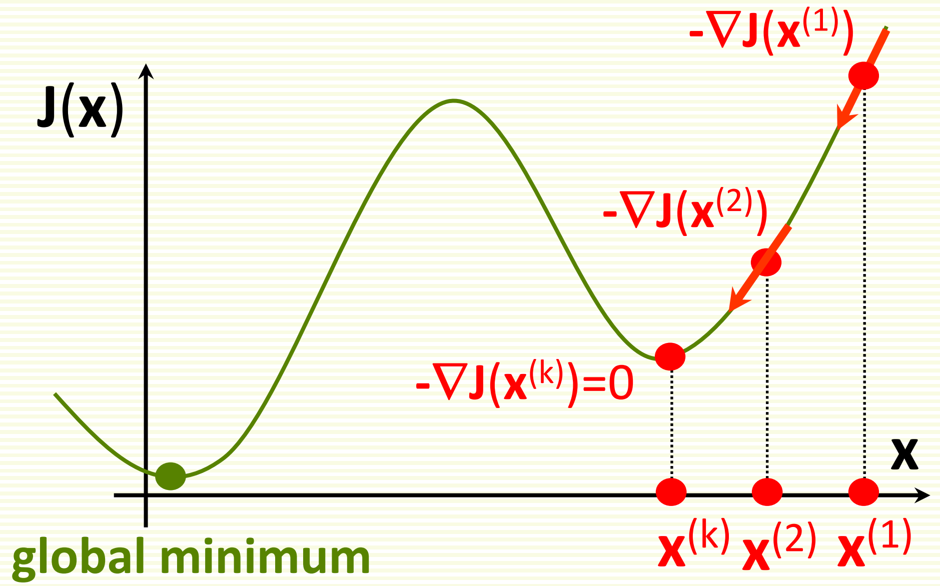
$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha \nabla \mathbf{J}(\mathbf{x}^{(k)})$

$\mathbf{k} = \mathbf{k} + 1$



Gradient Descent: Local Minimum

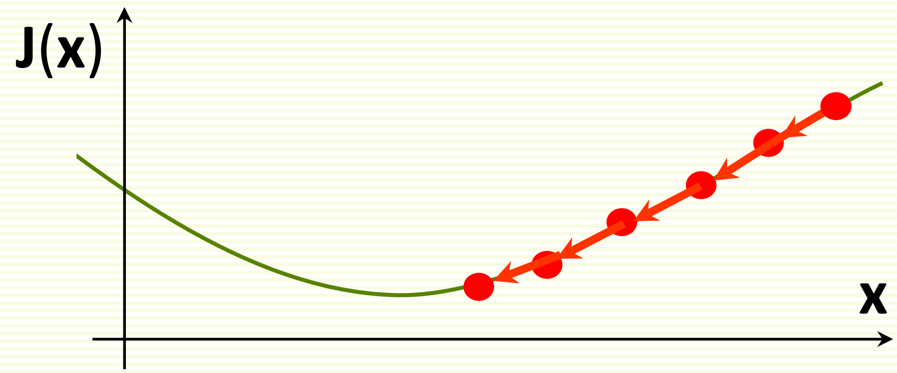
- Not guaranteed to find global minimum
  - gets stuck in local minimum



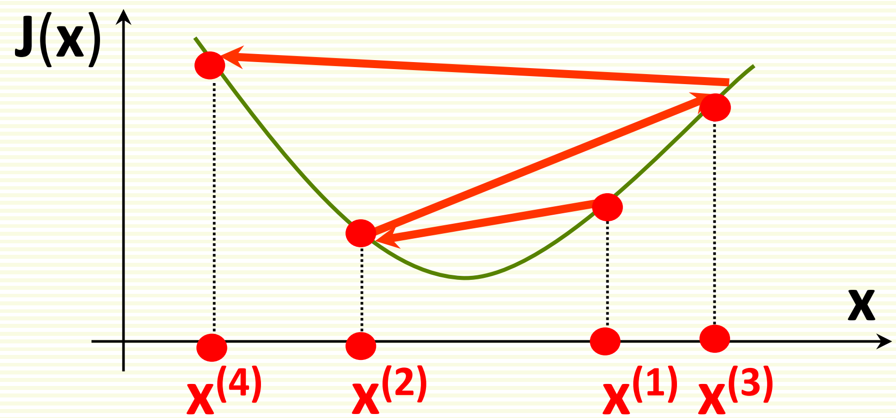
- Still gradient descent is very popular because it is simple and applicable to any differentiable function

How to Set Learning Rate α?

- If α too small, too many iterations to converge



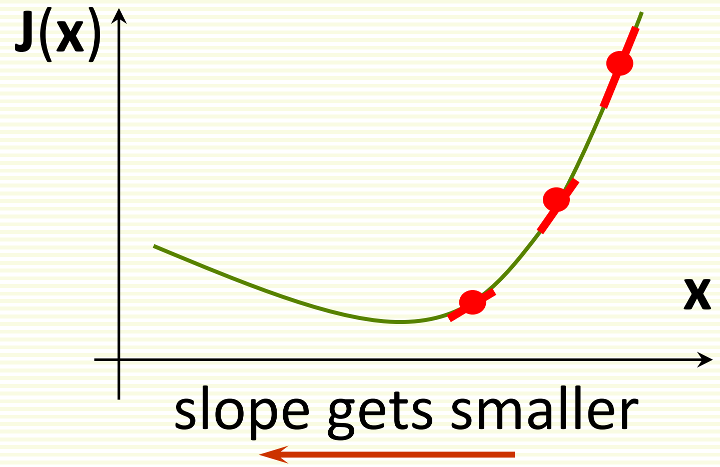
- If α too large, may overshoot the local minimum and possibly never even converge



- It helps to compute $\mathbf{J}(\mathbf{x})$ 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

$\mathbf{k} = 1$

$\mathbf{x}^{(1)}$ = any initial guess

choose α, ε

while $\alpha\|\nabla \mathbf{J}(\mathbf{x}^{(k)})\| > \varepsilon$

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

  $\mathbf{k} = \mathbf{k} + 1$

→

$\mathbf{k} = 1$

$\mathbf{x}^{(1)}$ = any initial guess

choose ε

while $\alpha\|\nabla \mathbf{J}(\mathbf{x}^{(k)})\| > \varepsilon$

  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

$\mathbf{k} = 1$

$\mathbf{x}^{(1)}$ = any initial guess

choose α, ε

while $\alpha \|\nabla \mathbf{J}(\mathbf{x}^{(k)})\| > \varepsilon$

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

$\quad \mathbf{k} = \mathbf{k} + 1$

$\rightarrow$

$\mathbf{x}$ = any initial guess

choose α, ε

while $\alpha \|\nabla \mathbf{J}(\mathbf{x})\| > \varepsilon$

$\quad \mathbf{x} = \mathbf{x} - \alpha \nabla \mathbf{J}(\mathbf{x})$

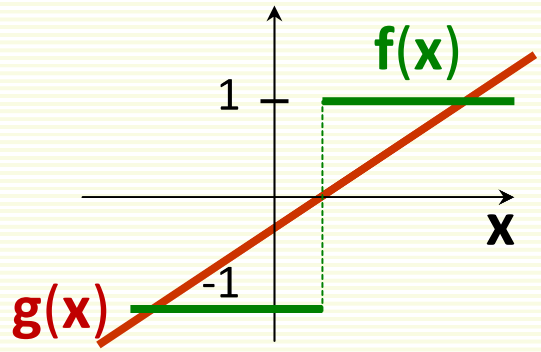
Advanced Optimization Methods

- There are more advanced gradient-based optimization methods
- Such as conjugate gradient
  - 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)

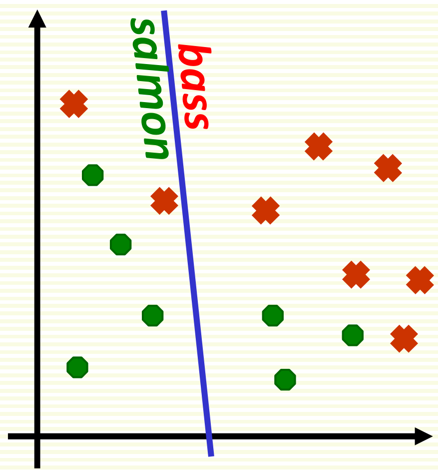
- Chose a *learning machine* **f**(**x**,**w**)
  - **w** are tunable weights, **x** is the input example
  - **f**(**x**,**w**) should output the correct class of sample **x**
  - use labeled samples to tune weights **w** so that **f**(**x**,**w**) give the correct class (correct **y**) for example **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

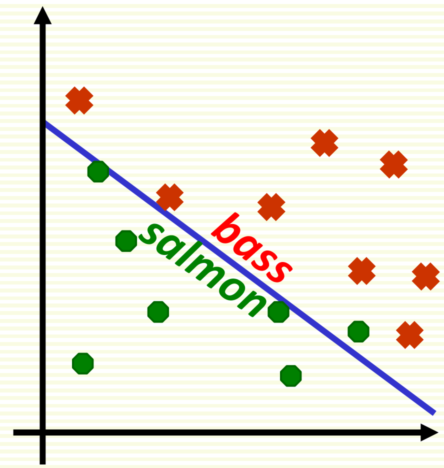


- First consider the two-class case
- We choose the following encoding:
  - **y** = 1 for the first class
  - **y** = -1 for the second class
- Linear classifier
  - linear function: $-\infty \leq \mathbf{w}_0+\mathbf{x}_1\mathbf{w}_1 + \ldots + \mathbf{x}_d\mathbf{w}_d \leq \infty$
  - we need **f**(**x**,**w**) to be either +1 or -1
  - let $\mathbf{g}(\mathbf{x},\mathbf{w}) = \mathbf{w}_0+\mathbf{x}_1\mathbf{w}_1 + \ldots + \mathbf{x}_d\mathbf{w}_d$
  - 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



bad boundary



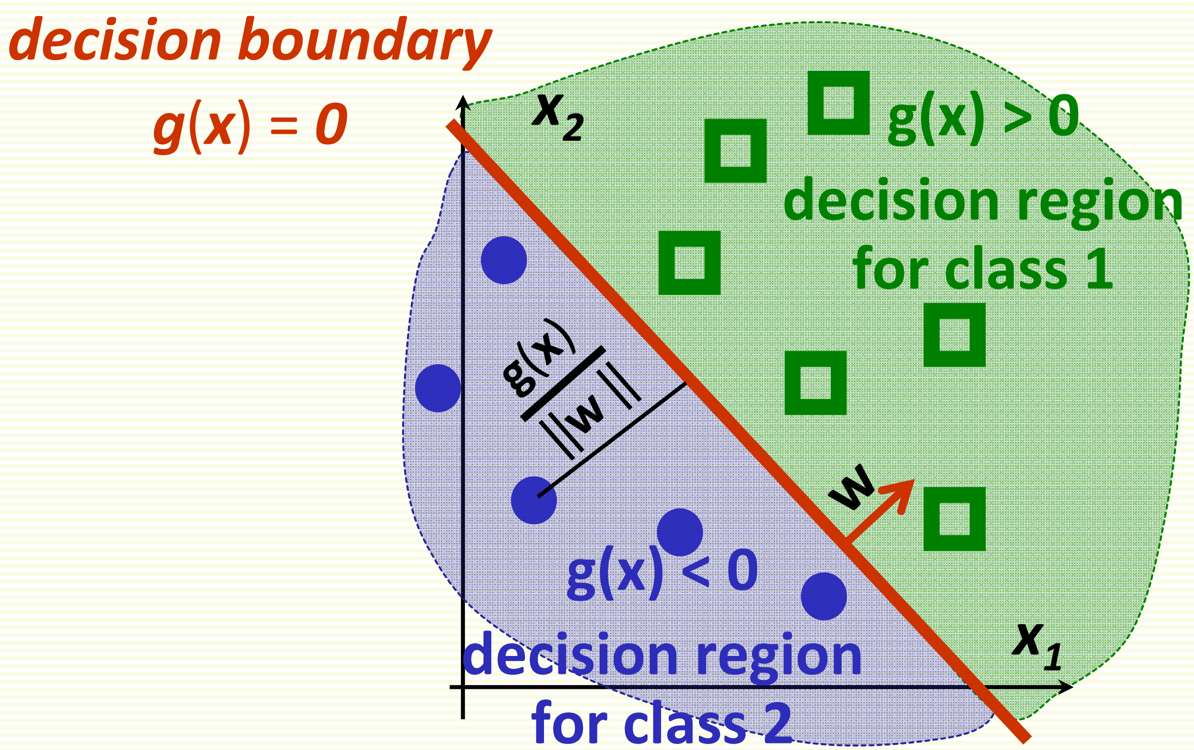
better boundary

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

More on Linear Discriminant Function (LDF)

- LDF: $\mathbf{g}(\mathbf{x},\mathbf{w}) = \mathbf{w}_0+\mathbf{x}_1\mathbf{w}_1 + \ldots + \mathbf{x}_d\mathbf{w}_d$
- Written using vector notation $\mathbf{g}(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + \mathbf{w}_0$

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

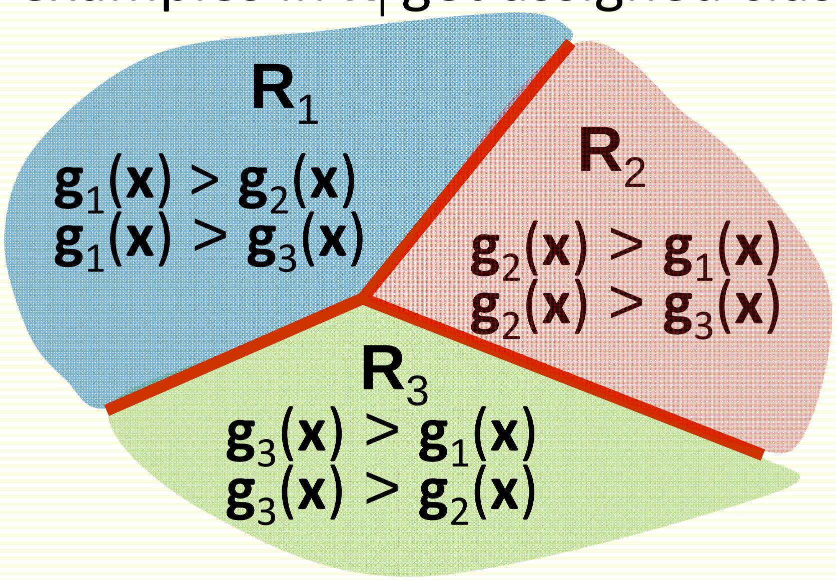
- We have **m** classes
- Define **m** linear discriminant functions

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

- Assign **x** to class **i** if

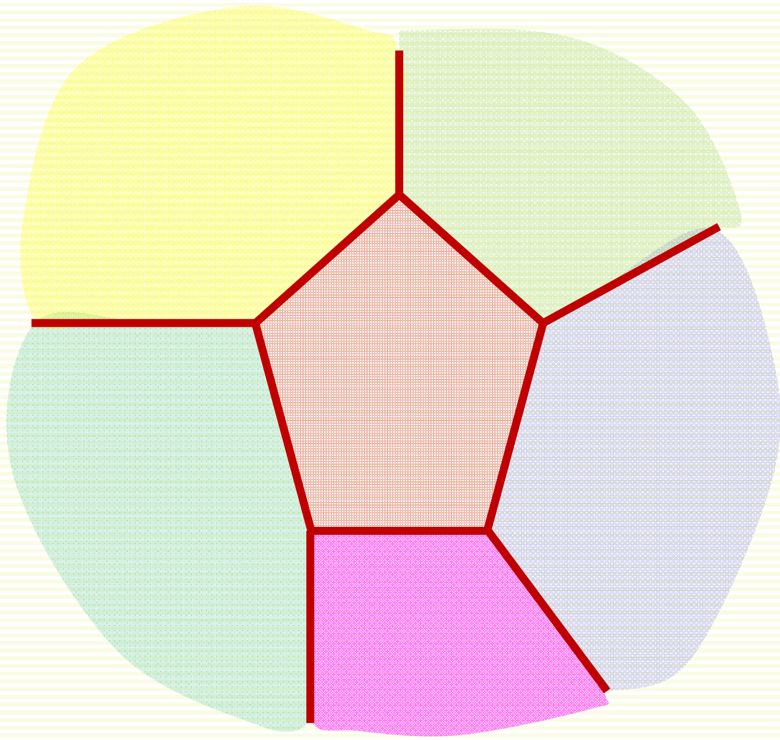
$$\mathbf{g}_i(\mathbf{x}) > \mathbf{g}_j(\mathbf{x}) \text{ for all } \mathbf{j} \neq \mathbf{i}$$

- Let $\mathbf{R}_i$ be the decision region for class **i**
  - That is all examples in $\mathbf{R}_i$ get assigned class **i**



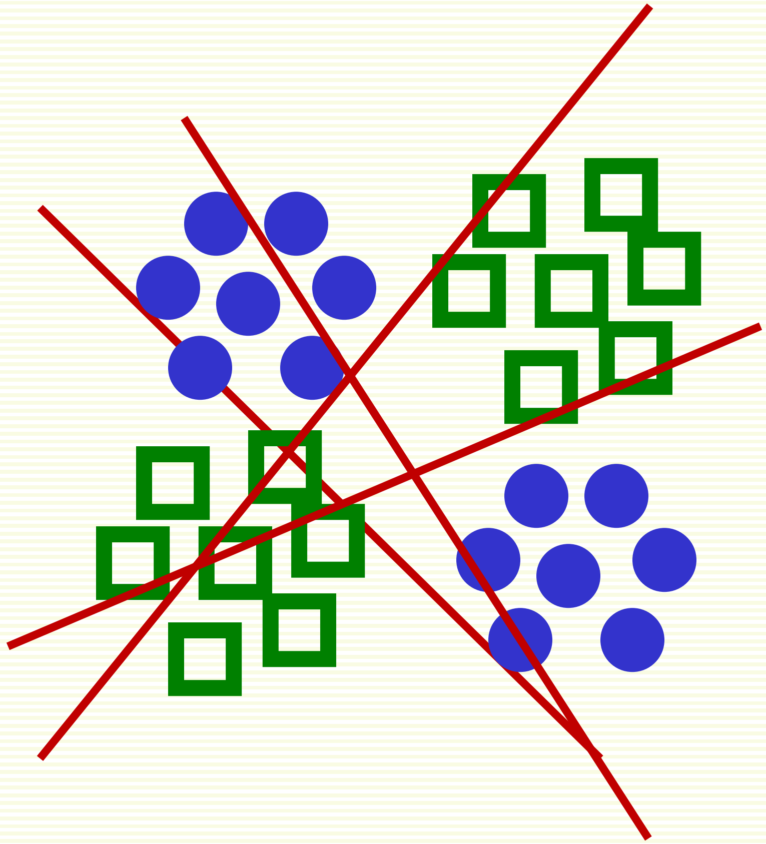
Multiple Classes

- 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



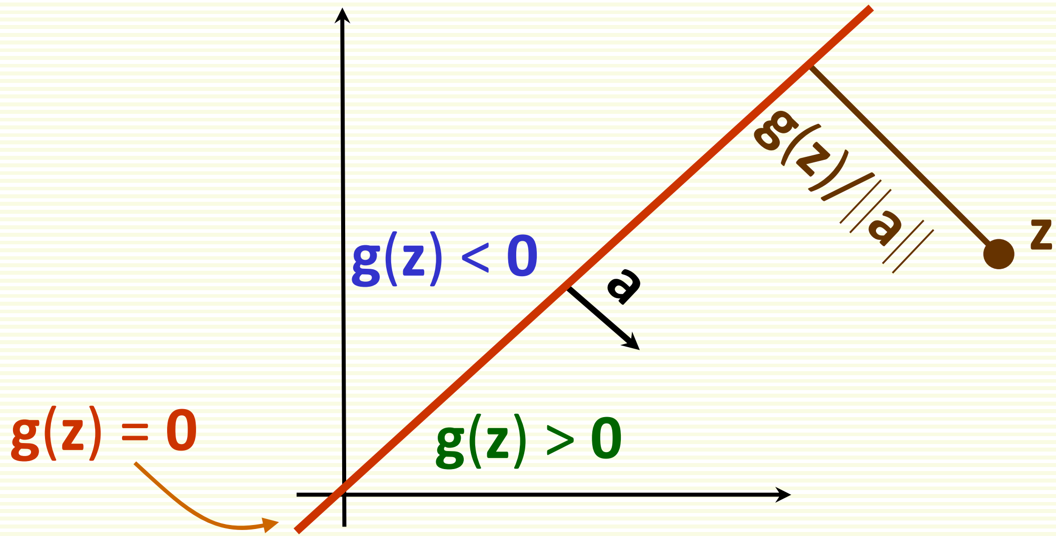
Fitting Parameters $\mathbf{w}$

- Linear discriminant function $\mathbf{g}(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + \mathbf{w}_0$
- Can rewrite it $\mathbf{g}(\mathbf{x}) = \underbrace{[\mathbf{w}_0 \quad \mathbf{w}^t]}_{\text{new weight vector } \boldsymbol{a}} \underbrace{\begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}}_{\text{new feature vector } \boldsymbol{z}} = \mathbf{a}^t\mathbf{z} = \mathbf{g}(\mathbf{z})$
- $\mathbf{z}$ is called augmented feature vector
- new problem equivalent to the old $\mathbf{g}(\mathbf{z}) = \mathbf{a}^t\mathbf{z}$

$$\mathbf{a} = \begin{bmatrix} \mathbf{w}_0 \\ \mathbf{w}_1 \\ \vdots \\ \mathbf{w}_d \end{bmatrix} \qquad \mathbf{z} = \begin{bmatrix} 1 \\ \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_d \end{bmatrix}$$

Augmented Feature Vector

- Feature augmenting is done to simplify notation
- From now on we assume that we have augmented feature vectors
  - given samples $\mathbf{x}^1, \ldots, \mathbf{x}^n$ convert them to augmented samples $\mathbf{z}^1, \ldots, \mathbf{z}^n$ by adding a new dimension of value 1
- $\mathbf{g(z) = a^t z}$



Training Error

- For the rest of the lecture, assume we have 2 classes
- Samples $\mathbf{z}^1,\ldots,\mathbf{z}^n$ some in class 1, some in class 2
- Use these samples to determine weights $\mathbf{a}$ in the discriminant function $\mathbf{g}(\mathbf{z}) = \mathbf{a}^t\mathbf{z}$
- Want to minimize number of misclassified samples
- Recall that $\begin{cases} \mathbf{g}(\mathbf{z}^i) > 0 & \Rightarrow \text{class 1} \\ \mathbf{g}(\mathbf{z}^i) < 0 & \Rightarrow \text{class 2} \end{cases}$
- 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 $\begin{cases} \mathbf{a}^t\mathbf{z}^i > 0 & \forall \mathbf{z}^i \text{ class 1} \\ \mathbf{a}^t\mathbf{z}^i < 0 & \forall \mathbf{z}^i \text{ class 2} \end{cases}$

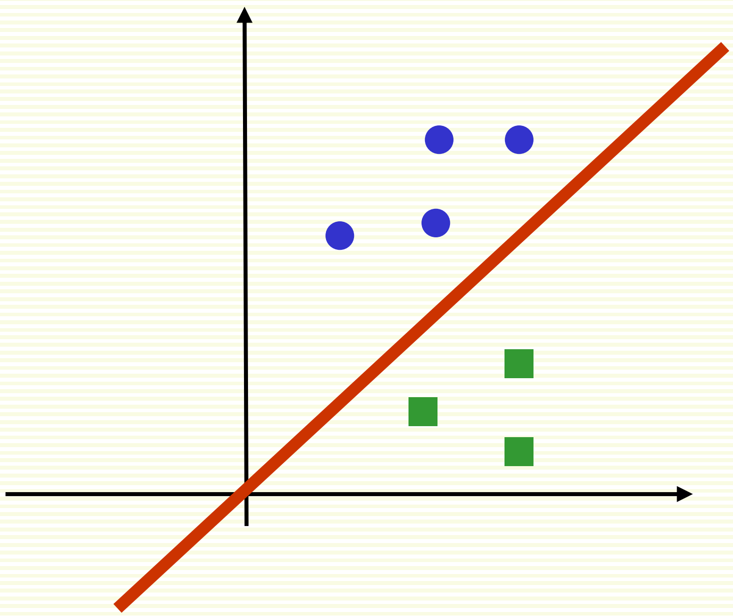
- Equivalently, training error is 0 if $\begin{cases} \mathbf{a}^t\mathbf{z}^i > 0 & \forall \mathbf{z}^i \text{ class 1} \\ \mathbf{a}^t(-\mathbf{z}^i) > 0 & \forall \mathbf{z}^i \text{ class 2} \end{cases}$

- Problem "normalization":
  1. replace all examples $\mathbf{z}^i$ from class 2 by $-\mathbf{z}^i$
  2. seek weights $\mathbf{a}$ 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 $\mathbf{x}^1, \ldots \mathbf{x}^n$ can also be linearly separated

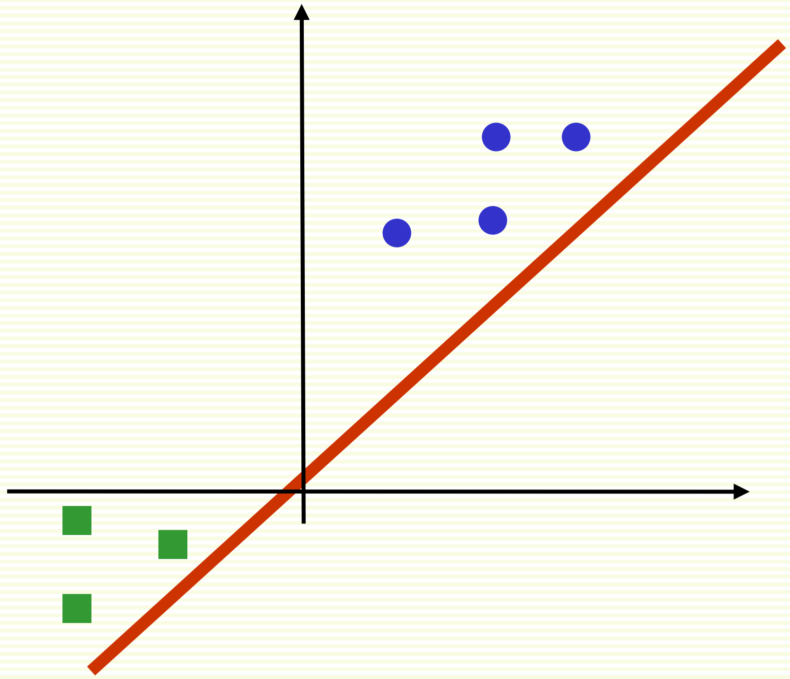
Effect of Normalization

before normalization



seek a hyperplane that separates samples from different categories

after normalization

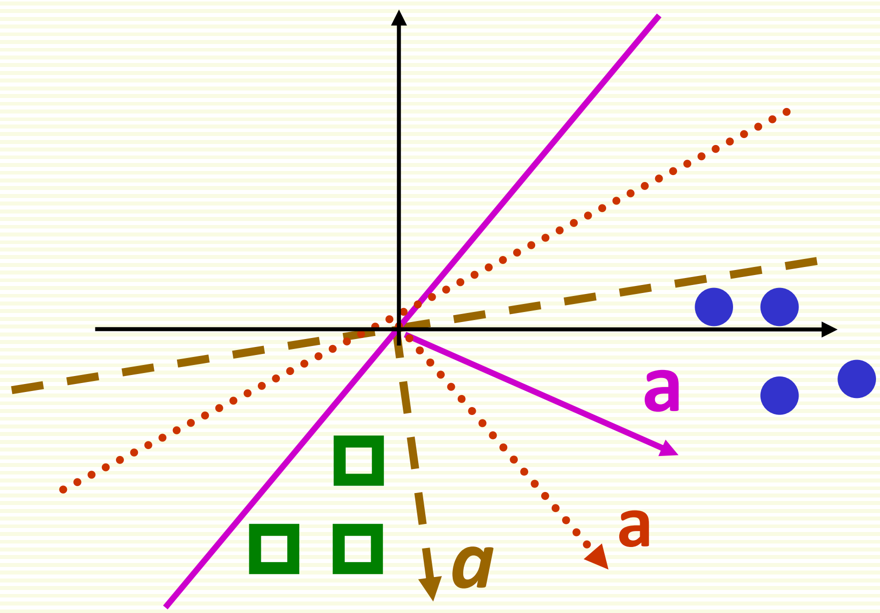


seek hyperplane that puts normalized samples on the same (positive) side

Solution Region

- Find weight vector **a** s.t. for all samples $\mathbf{z}^1,\ldots,\mathbf{z}^n$

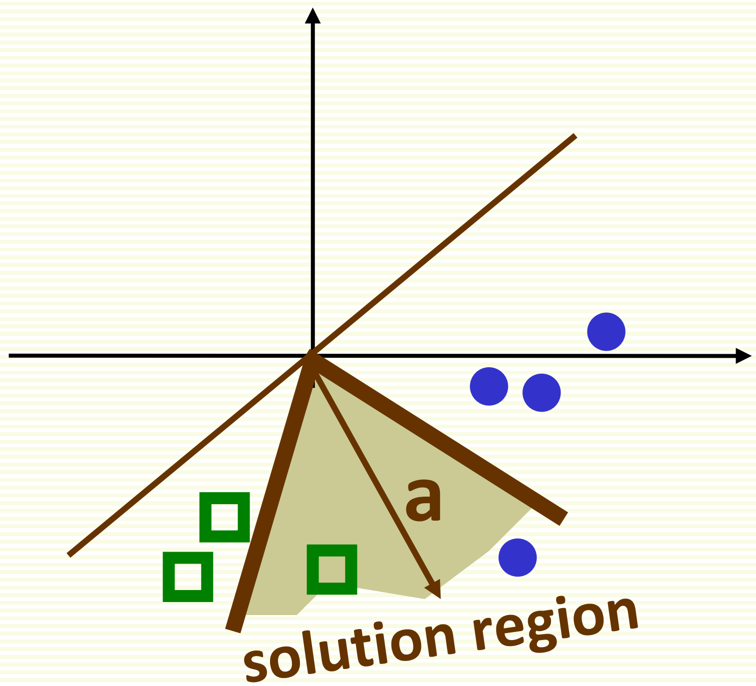
$$\mathbf{a}^t\mathbf{z}^i = \sum_{k=0}^{d} \mathbf{a}_k \mathbf{z}_d^i > \mathbf{0}$$



- 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

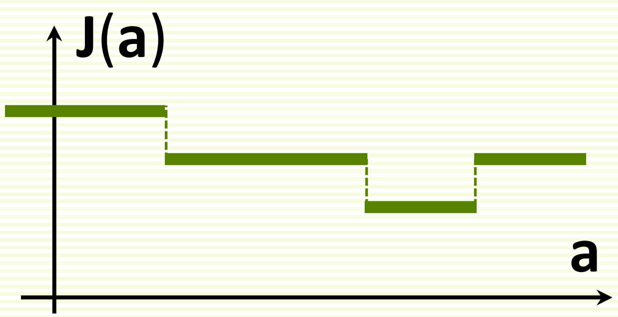
- Find weight vector **a** s.t. $\forall \mathbf{z}^1, \dots, \mathbf{z}^n$, $\mathbf{a}^t \mathbf{z}^i > 0$
- Design a criterion function $\mathbf{J}(\mathbf{a})$, which is minimum when **a** is a solution vector
- Let $\mathbf{Z}(\mathbf{a})$ be the set of examples misclassified by **a**

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

- Natural choice: number of misclassified examples

$$\mathbf{J}(\mathbf{a}) = |\mathbf{Z}(\mathbf{a})|$$

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

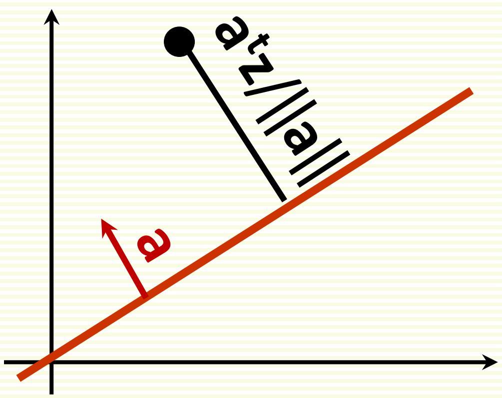


Perceptron Criterion Function

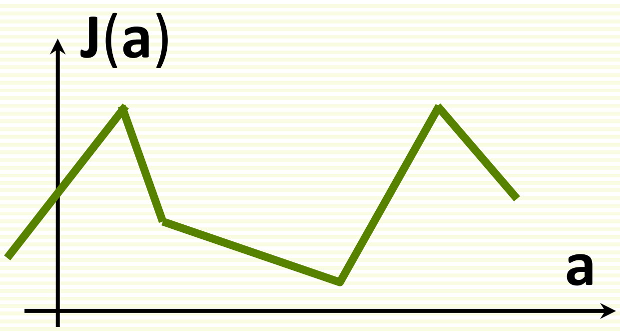
- Better choice: Perceptron criterion function

$$J_p(\mathbf{a}) = \sum_{\mathbf{z} \in Z(\mathbf{a})} \left(-\mathbf{a}^t \mathbf{z}\right)$$

- If $\mathbf{z}$ is misclassified, $\mathbf{a}^t\mathbf{z} < 0$
- Thus $\mathbf{J}(\mathbf{a}) \geq 0$
- $\mathbf{J}_p(\mathbf{a})$ is proportional to the sum of distances of misclassified examples to decision boundary



- $\mathbf{J}_p(\mathbf{a})$ is piecewise linear and suitable for gradient descent



Optimizing with Gradient Descent

$$\mathbf{J_p}(\mathbf{a}) = \sum_{\mathbf{z} \in \mathbf{Z}(\mathbf{a})} \left(-\mathbf{a}^t \mathbf{z}\right)$$

- Gradient of $\mathbf{J}_p(\mathbf{a})$ is $\nabla \mathbf{J_p}(\mathbf{a}) = \sum_{\mathbf{z} \in \mathbf{Z}(\mathbf{a})} (-\mathbf{z})$
  - 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 $\mathbf{J}_p(\mathbf{a})$ is:

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

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

Perceptron Single Sample Rule

- Gradient decent single sample rule for $\mathbf{J}_p(\mathbf{a})$ is

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

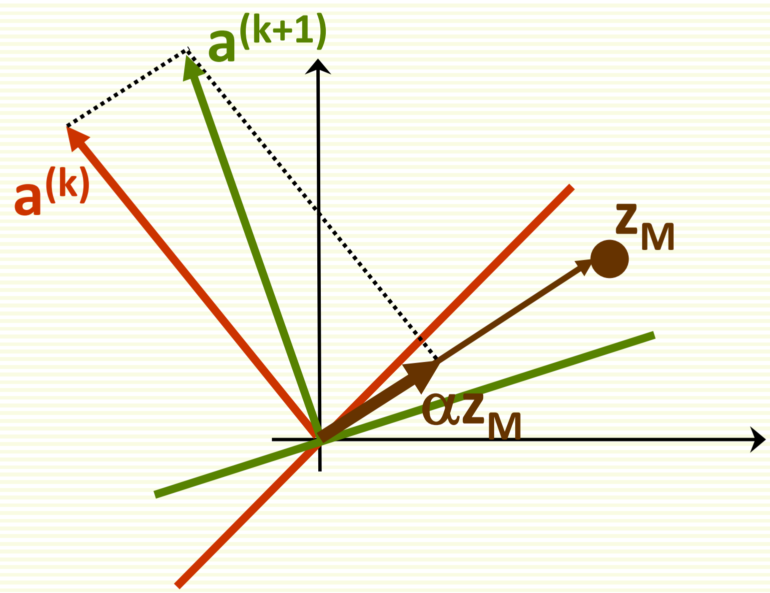
  - $\mathbf{z}_M$ is one sample misclassified by $\mathbf{a}^{(k)}$
  - must have a consistent way to visit samples

- Geometric Interpretation:

- $\mathbf{z}_M$ misclassified by $\mathbf{a}^{(k)}$

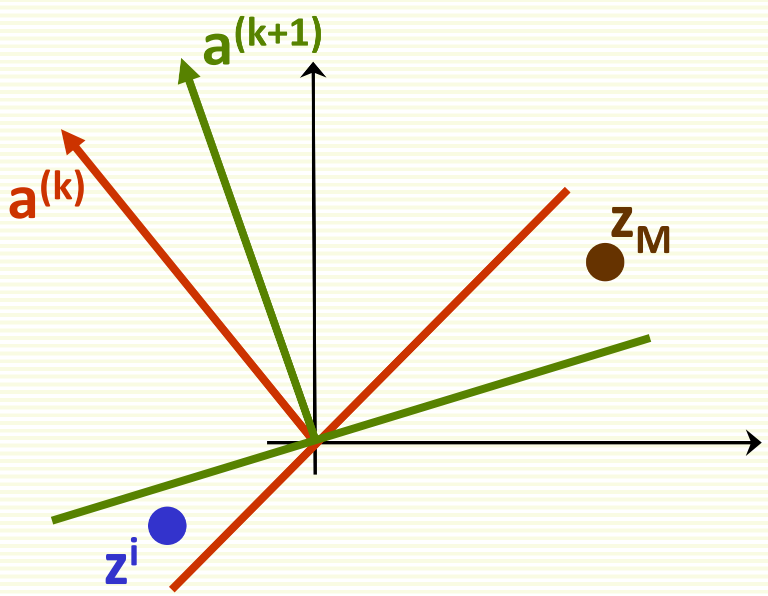
$$\left(\mathbf{a}^{(k)}\right)^t \mathbf{z}_M \le 0$$

- $\mathbf{z}_M$ is on the wrong side of decision boundary
- adding $\alpha \cdot \mathbf{z}_M$ to a moves decision boundary in the right direction

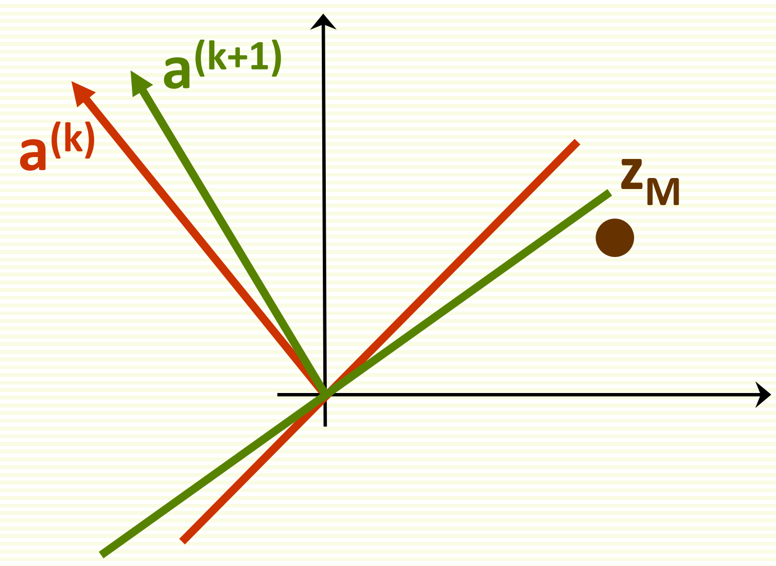


Perceptron Single Sample Rule

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



if α is too small, $\mathbf{z}_M$ is still 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)*	*A*
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)*	*A*

- 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)*	*A*
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)*	*A*

- convert samples $\mathbf{x}^1,\ldots,\mathbf{x}^n$ to augmented samples $\mathbf{z}^1,\ldots,\mathbf{z}^n$ 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)*	*A*
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)*	*A*

- Replace all examples from class 2 by their negative

$$\mathbf{z}^i \longrightarrow -\mathbf{z}^i$$

- Seek weight vector **a** s.t. $\mathbf{a}^t\mathbf{z}^i > 0$ for all $\mathbf{z}^i$

Apply Single Sample Rule

	features					grade
name	***extra***	***good attendance?***	***tall?***	***sleeps in class?***	***chews gum?***	
Jane	*1*	*yes (1)*	*yes (1)*	*no (-1)*	*no (-1)*	*A*
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)*	*A*

- 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 $\mathbf{a}^t \mathbf{z}^i = \sum_{\mathbf{k}=0}^{4} \mathbf{a}_k \mathbf{z}_k^i < 0$

Apply Single Sample Rule

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

name	$\mathbf{a}^t\mathbf{z}$	***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

$$\mathbf{a}^{(2)} = \mathbf{a}^{(1)} + \mathbf{z}_{\mathbf{M}} = \begin{bmatrix} 0.25 & 0.25 & 0.25 & 0.25 & 0.25 \end{bmatrix} +$$
$$+ \begin{bmatrix} -1 & -1 & -1 & -1 & -1 \end{bmatrix} =$$
$$= \begin{bmatrix} -0.75 & -0.75 & -0.75 & -0.75 & -0.75 \end{bmatrix}$$

Apply Single Sample Rule

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

name	$\mathbf{a}^t\mathbf{z}$	*misclassified?*
Mary	*-0.75*(-1)-0.75*1 -0.75 *1 -0.75 *1 -0.75*(-1) <0*	*yes*

- new weights

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

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

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

Apply Single Sample Rule

$$\boldsymbol{a}^{(3)} = [-1.75 \quad 0.25 \quad 0.25 \quad 0.25 \quad -1.75]$$

name	$\mathbf{a}^t\mathbf{z}$	*misclassified?*
Peter	*-1.75 *1 +0.25* 1+0.25* (-1) +0.25 *(-1)-1.75*1 <0*	*yes*

- new weights

$$\mathbf{a}^{(4)} = \mathbf{a}^{(3)} + \mathbf{z_M} = [-1.75 \quad 0.25 \quad 0.25 \quad 0.25 \quad -1.75] +$$

$$+ [1 \quad 1 \quad -1 \quad -1 \quad 1] =$$

$$= [-0.75 \quad 1.25 \quad -0.75 \quad -0.75 \quad -0.75]$$

Single Sample Rule: Convergence

$$\mathbf{a}^{(4)} = [-0.75 \quad 1.25 \quad -0.75 \quad -0.75 \quad -0.75]$$

name	$\mathbf{a}^t\mathbf{z}$	***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**

$$\mathbf{g}(\mathbf{x}) = 1.25x_1 - 0.75\mathbf{x}_2 - 0.75\mathbf{x}_3 - 0.75\mathbf{x}_4 - 0.75$$

Final Classifier

- Trained LDF: $\mathbf{g}(\mathbf{x}) = 1.25x_1 - 0.75\mathbf{x}_2 - 0.75\mathbf{x}_3 - 0.75\mathbf{x}_4 - 0.75$
- Leads to classifier:

$$1.25x_1 - 0.75\mathbf{x}_2 - 0.75\mathbf{x}_3 - 0.75\mathbf{x}_4 > 0.75 \Rightarrow \text{grade } \mathbf{A}$$

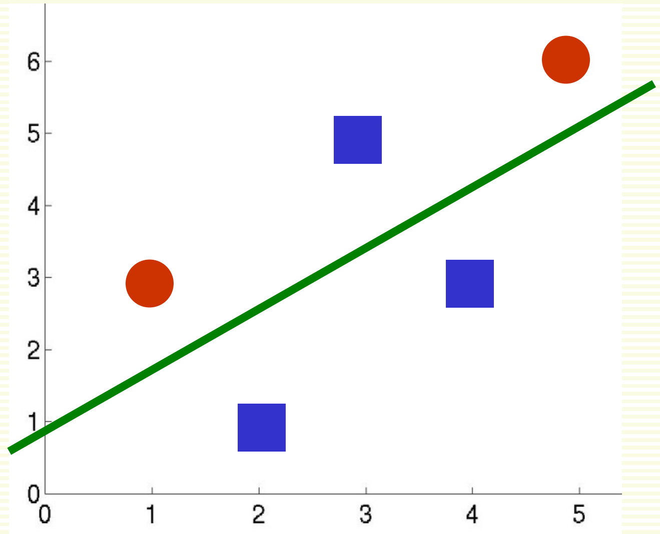
good attendance **tall** **sleeps in class** **chews gum**

- This is just *one* possible solution vector
- With $\mathbf{a}^{(1)}=[0,0.5, 0.5, 0, 0]$, solution is $[-1,1.5, -0.5, -1, -1]$

$$1.5x_1 - 0.5\mathbf{x}_2 - \mathbf{x}_3 - \mathbf{x}_4 > 1 \Rightarrow \text{grade } \mathbf{A}$$

  - In this solution, being tall is the least important feature

Non-Linearly Separable Case

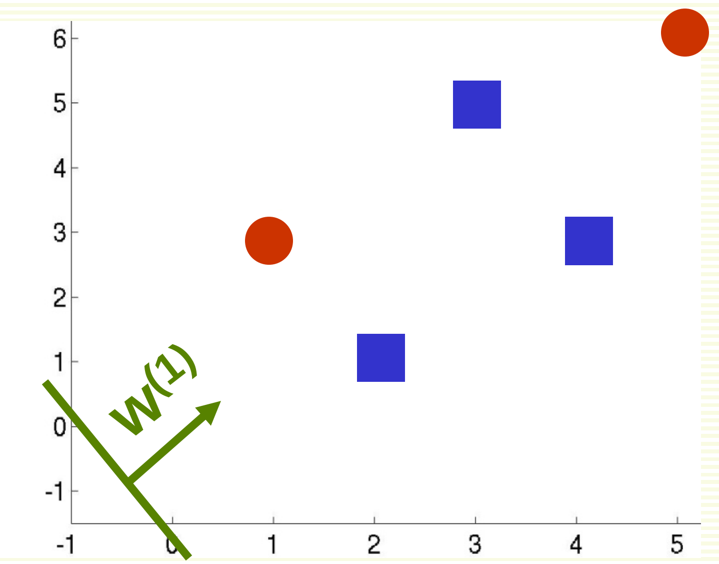


- Suppose we have examples:
  - class 1: [2,1], [4,3], [3,5]
  - class 2: [1,3] , [5,6]
  - not linearly separable
- Still would like to get approximate separation
- Good line choice is shown in green
- Let us run gradient descent
  - Add extra feature and "normalize"

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

Non-Linearly Separable Case

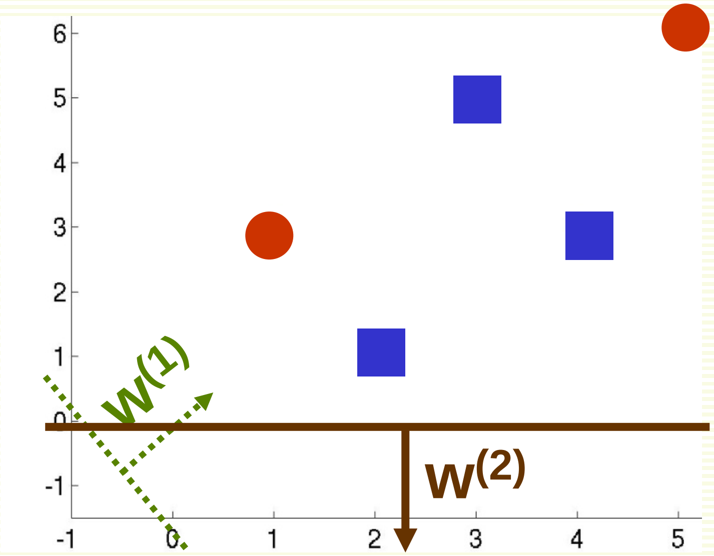
- single sample perceptron rule
- Initial weights $\mathbf{a}^{(1)} = [1\ \ 1\ \ 1]$
- This is line $\mathbf{x}_1 + \mathbf{x}_2 + 1 = 0$
- Use fixed learning rate $\alpha = 1$
- Rule is: $\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \mathbf{z}_M$



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

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

Non-Linearly Separable Case



- $\mathbf{a}^{(1)} = [1 \;\; 1 \;\; 1]$
- rule is: $\mathbf{a}^{(k+1)} = \mathbf{a}^{(k)} + \mathbf{z}_M$

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

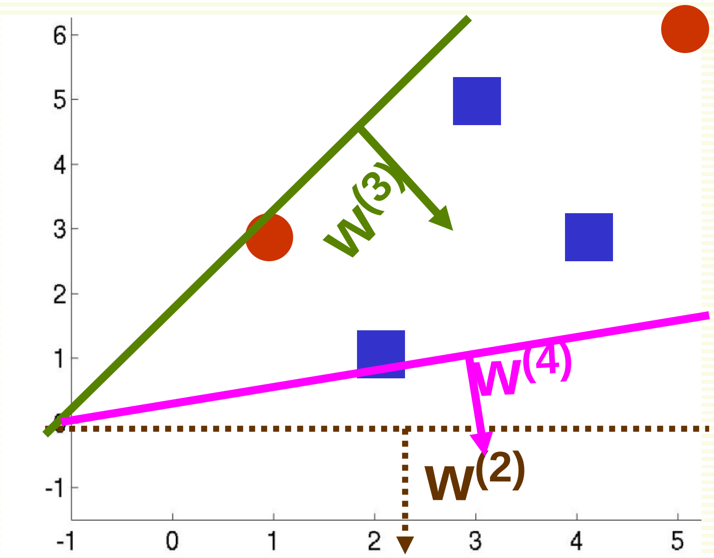
- $\mathbf{a}^t\mathbf{z}^4 = [1\;1\;1] \cdot [-1\;-1\;-3]^t = -5 < 0$
- *Update:* $\mathbf{a}^{(2)} = \mathbf{a}^{(1)} + \mathbf{z}_M = [1 \;\; 1 \;\; 1] + [-1 \;\; -1 \;\; -3] = [0 \;\; 0 \;\; -2]$

- $\mathbf{a}^t\mathbf{z}^5 = [0\;0\;-2] \cdot [-1\;-5\;-6]^t = 12 > 0$
- $\mathbf{a}^t\mathbf{z}^1 = [0\;0\;-2] \cdot [1\;2\;1]^t < 0$
- *Update:* $\mathbf{a}^{(3)} = \mathbf{a}^{(2)} + \mathbf{z}_M = [0 \;\; 0 \;\; -2] + [1 \;\; 2 \;\; 1] = [1 \;\; 2 \;\; -1]$

Non-Linearly Separable Case

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

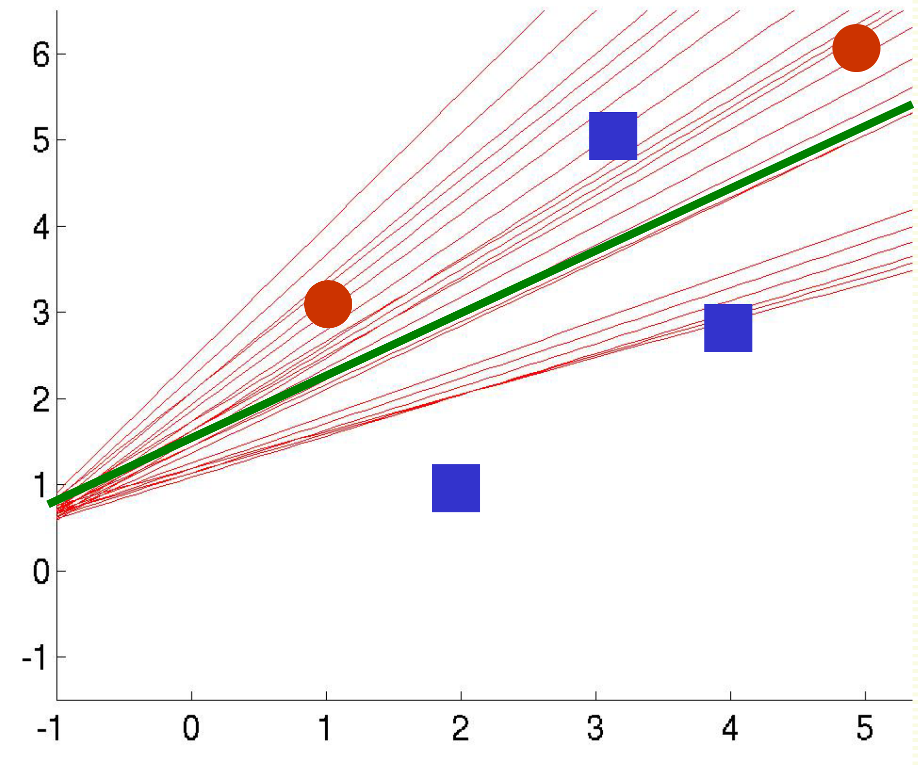
$$\mathbf{z}^1 = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} \quad \mathbf{z}^2 = \begin{bmatrix} 1 \\ 4 \\ 3 \end{bmatrix} \quad \mathbf{z}^3 = \begin{bmatrix} 1 \\ 3 \\ 5 \end{bmatrix} \quad \mathbf{z}^4 = \begin{bmatrix} -1 \\ -1 \\ -3 \end{bmatrix} \quad \mathbf{z}^5 = \begin{bmatrix} -1 \\ -5 \\ -6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



- $\mathbf{a}^t\mathbf{z}^2 = [1\;4\;3] \cdot [1 \;\; 2\; -1]^t = 6 > 0$
- $\mathbf{a}^t\mathbf{z}^3 = [1\;3\;5] \cdot [1 \;\; 2\; -1]^t = 2 > 0$
- $\mathbf{a}^t\mathbf{z}^4 = [-1\;-1\;-3] \cdot [1 \;\; 2\; -1]^t = 0$
- *Update:* $\mathbf{a}^{(4)} = \mathbf{a}^{(3)} + \mathbf{z}_M = [1 \;\; 2 \;\; -1] + [-1 \;\; -1 \;\; -3] = [0 \;\; 1 \;\; -4]$

Non-Linearly Separable Case

- We can continue this forever
  - there is no solution vector **a** satisfying for all $\mathbf{a}^t\mathbf{z}_i > 0$ 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
     - $\alpha \to 0$ as $\mathbf{k} \to \infty$
     - example, inverse linear: $\alpha = \mathbf{c}/\mathbf{k}$, 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

$\mathbf{a}^t\mathbf{z}^i > 0$ for all samples $\mathbf{z}^i$

solve system of linear inequalities

↓

$\mathbf{a}^t\mathbf{z}^i = \boldsymbol{b}_i$ for all samples $\mathbf{z}^i$

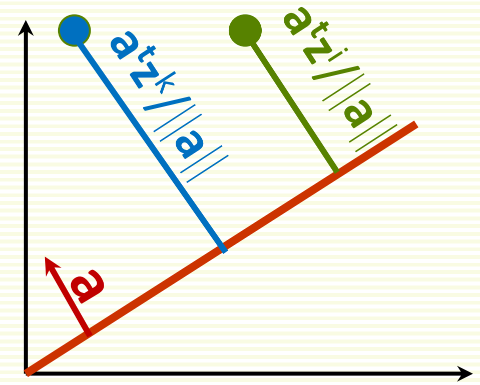
solve system of linear equations

- MSE procedure
  - choose positive constants $\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_n$
  - try to find weight vector **a** s.t. $\mathbf{a}^t\mathbf{z}^i = \mathbf{b}_i$ for all samples $\mathbf{z}^i$
  - if succeed, then **a** is a solution because $\mathbf{b}_i$'s are positive
  - consider all the samples (not just the misclassified ones)

MSE: Margins

- By setting $\mathbf{a}^t\mathbf{z}^i = \mathbf{b}_i$, we expect $\mathbf{z}^i$ to be at a relative distance $\mathbf{b}_i$ from the separating hyperplane
- Thus $\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_n$ are expected relative distances of examples from the separating hyperplane
- Should make $\mathbf{b}_i$ small if sample $\mathbf{i}$ is expected to be near separating hyperplane, and make $\mathbf{b}_i$ 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 $\begin{cases} \mathbf{a}^t\mathbf{z}^1 = \mathbf{b}_1 \\ \vdots \\ \mathbf{a}^t\mathbf{z}^n = \mathbf{b}_n \end{cases}$
- Using matrix notation:

$$\underbrace{\begin{bmatrix} \mathbf{z}_0^1 & \mathbf{z}_1^1 & \cdots & \mathbf{z}_d^1 \\ \mathbf{z}_0^2 & \mathbf{z}_1^2 & \cdots & \mathbf{z}_d^2 \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ \mathbf{z}_0^n & \mathbf{z}_1^n & \cdots & \mathbf{z}_d^n \end{bmatrix}}_{\mathbf{Z}} \underbrace{\begin{bmatrix} \mathbf{a}_0 \\ \mathbf{a}_1 \\ \vdots \\ \mathbf{a}_d \end{bmatrix}}_{\mathbf{a}} = \underbrace{\begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \vdots \\ \mathbf{b}_n \end{bmatrix}}_{\mathbf{b}}$$

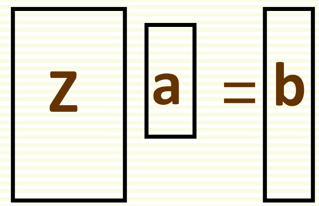
- Solve a linear system **Za** = **b**

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 $\mathbf{Z}^{-1}$ exists
  - $\mathbf{a} = \mathbf{Z}^{-1}\,\mathbf{b}$
  - (number of samples) = (number of features + 1)
- if happens, guaranteed to find separating hyperplane
  - but almost never happens in practice

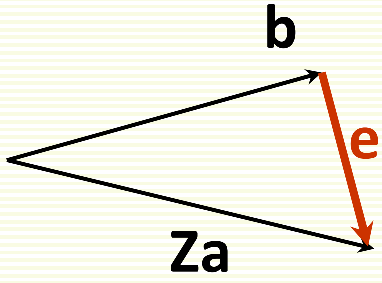
MSE:Approximate Solution

- 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:

$$J_s(\mathbf{a}) = \|\mathbf{Za} - \mathbf{b}\|^2 = \sum_{i=1}^{n} \left(\mathbf{a}^t \mathbf{z}^i - \mathbf{b}_i\right)^2$$

- Can be optimized exactly

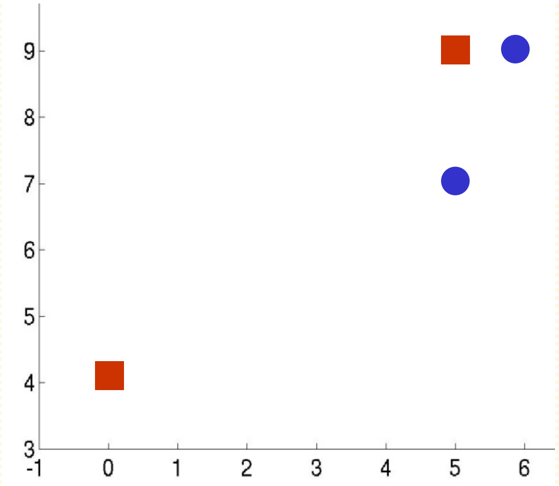
MSE: Optimizing $J_S(\mathbf{a})$

$$J_s(\mathbf{a}) = \|\mathbf{Za} - \mathbf{b}\|^2 = \sum_{i=1}^{n} \left(\mathbf{a}^t \mathbf{z}^i - \mathbf{b}_i\right)^2$$

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

MSE: Example

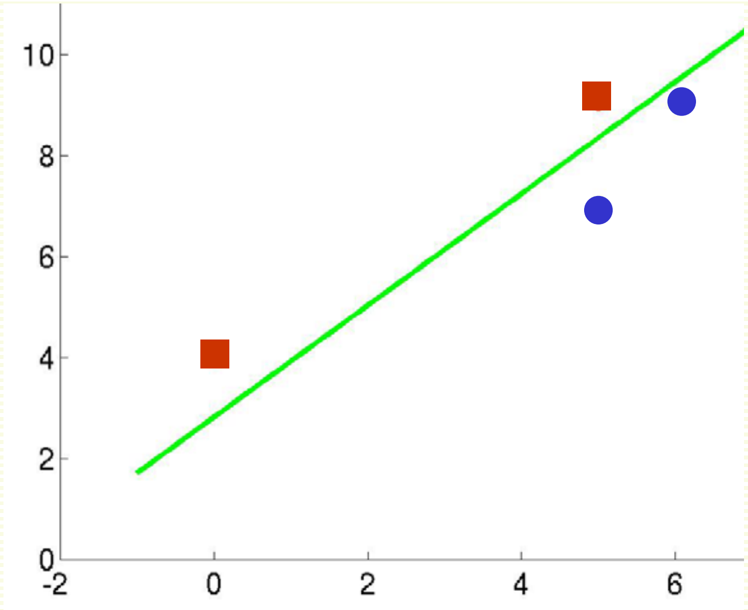
- Class 1: (6 9), (5 7)
- Class 2: (5 9), (0 4)
- Add extra feature and "normalize"



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

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

MSE: Example



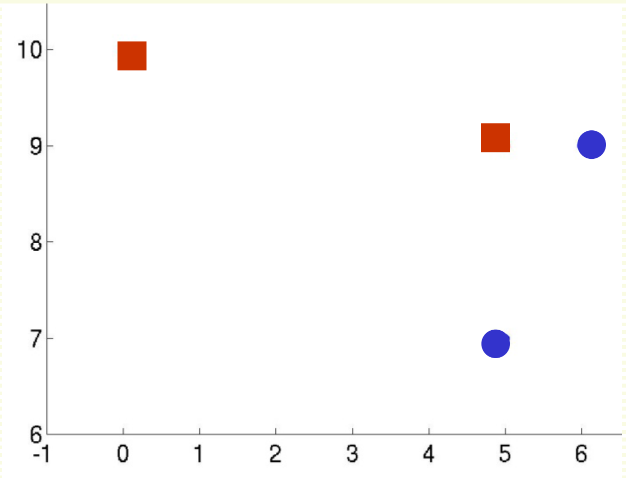
- Choose $\mathbf{b}=\begin{bmatrix}1\\1\\1\\1\end{bmatrix}$
- Use **a=Z\b** to solve in Matlab

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

- Note **a** is an approximation since $\mathbf{Za}=\begin{bmatrix}0.4\\1.3\\0.6\\1.1\end{bmatrix}\neq\begin{bmatrix}1\\1\\1\\1\end{bmatrix}$
- Gives a separating hyperplane since $\mathbf{Za} > 0$

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

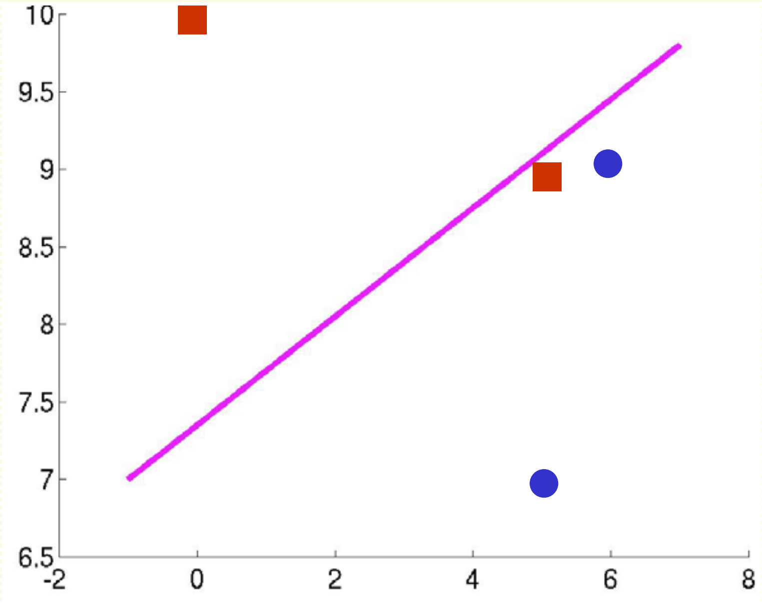


$$\mathbf{z}^1 = \begin{bmatrix} 1 \\ 6 \\ 9 \end{bmatrix} \quad \mathbf{z}^2 = \begin{bmatrix} 1 \\ 5 \\ 7 \end{bmatrix} \quad \mathbf{z}^3 = \begin{bmatrix} -1 \\ -5 \\ -9 \end{bmatrix} \quad \mathbf{z}^4 = \begin{bmatrix} -1 \\ 0 \\ -10 \end{bmatrix}$$

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

MSE: Another Example Cont.

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



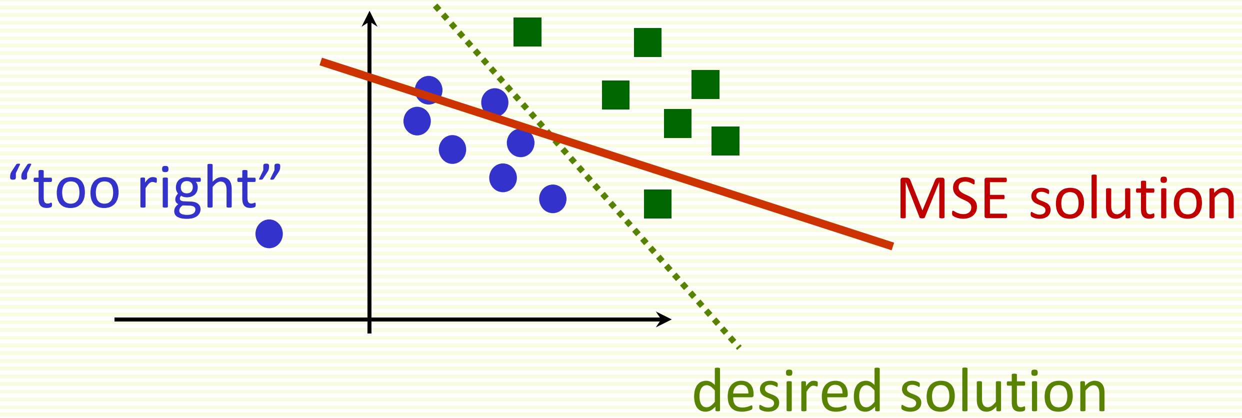
- Solve $\mathbf{a} = \mathbf{Z} \backslash \mathbf{b} = \begin{bmatrix} 3.2 \\ 0.2 \\ -0.4 \end{bmatrix}$

- $\mathbf{Za} = \begin{bmatrix} 0.2 \\ 0.9 \\ -0.04 \\ 1.16 \end{bmatrix} \neq \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$

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

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

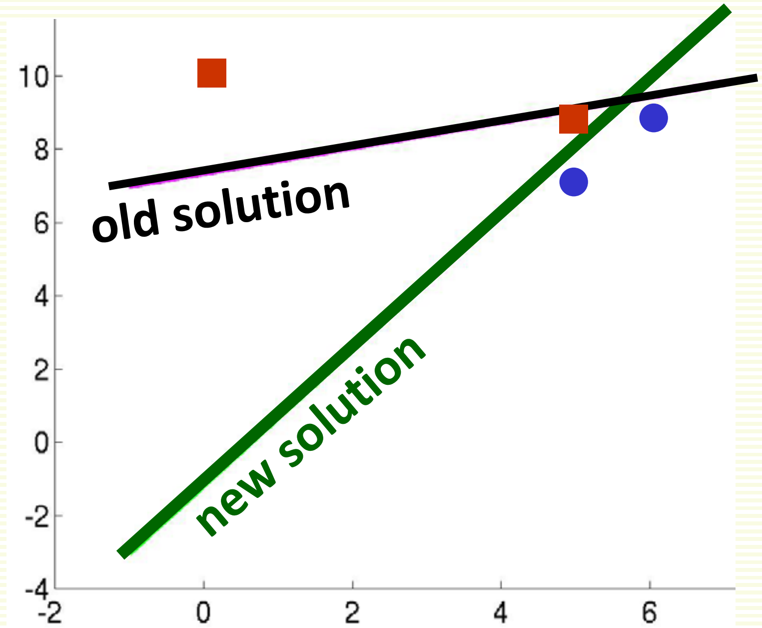


- No problems with convergence though, both in separable and non-separable cases

MSE: Another Example Cont.

- If we know that 4^{th} point is far from separating hyperplane
  - in practice can look at points which are furthest from the decision boundary

$$\mathbf{Za} = \begin{bmatrix} 0.2 \\ 0.9 \\ -0.04 \\ 1.16 \end{bmatrix}$$



- Set $\mathbf{b}_i$ larger for such points: $\mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 10 \end{bmatrix}$

- Solve $\mathbf{a}=\mathbf{Z}\backslash\mathbf{b} = \begin{bmatrix} -1.1 \\ 1.7 \\ -0.9 \end{bmatrix}$

- $\mathbf{Za} = \begin{bmatrix} 0.9 \\ 1.0 \\ 0.8 \\ 10.0 \end{bmatrix} \neq \begin{bmatrix} 1 \\ 1 \\ 1 \\ 10 \end{bmatrix} > 0$, therefore gives a separating hyperplane

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