## CS9840

# Learning and Computer Vision Prof. Olga Veksler

## Lecture 7 Linear Machines

## Today

- 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
- Generalized Linear Classifier
- Gradient Descent Based learning

## **Optimization**

- How to minimize a function of a single variable
   J(x) = (x-5)<sup>2</sup>
- 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**

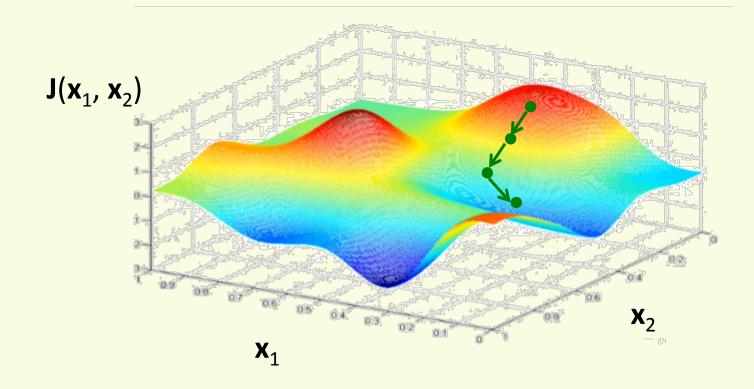
- How to minimize a function of many variables
   J(x) = J(x<sub>1</sub>,..., x<sub>d</sub>)
- From calculus, take partial derivatives, set them to 0

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

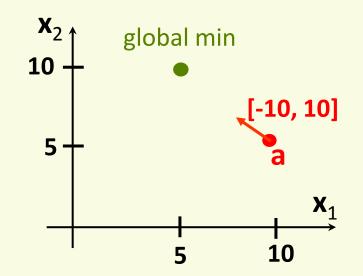
#### **Gradient Direction in 2D**

• 
$$J(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 - 5)^2 + (\mathbf{x}_2 - 10)^2$$

• 
$$\frac{\partial}{\partial \mathbf{x}_1} \mathbf{J}(\mathbf{x}) = \mathbf{2}(\mathbf{x}_1 - \mathbf{5})$$
  
•  $\frac{\partial}{\partial \mathbf{x}_2} \mathbf{J}(\mathbf{x}) = \mathbf{2}(\mathbf{x}_2 - \mathbf{10})$ 

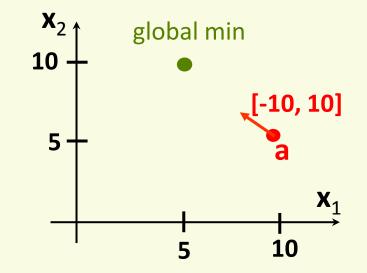
• Let **a** = [10, 5]

• 
$$-\frac{\partial}{\partial x_1} J(a) = -10$$
  
•  $-\frac{\partial}{\partial x_2} J(a) = 10$ 



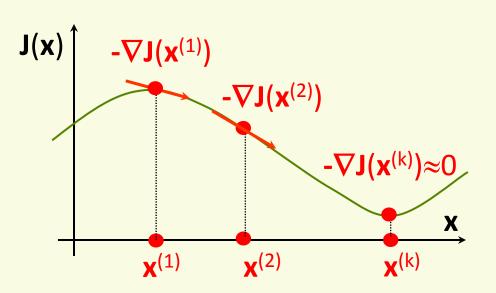
### **Gradient Descent: Step Size**

- $J(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 5)^2 + (\mathbf{x}_2 10)^2$
- Which step size to take?
- Controlled by parameter  $\alpha$ 
  - 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



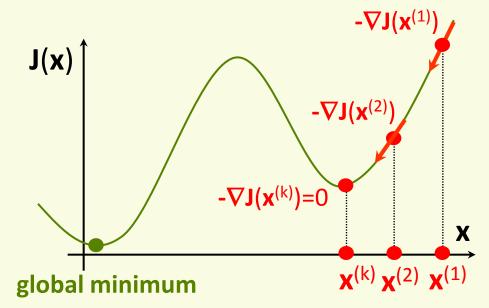
#### **Gradient Descent Algorithm**

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



#### **Gradient Descent: Local Minimum**

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



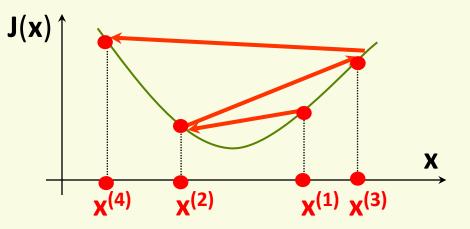
• Still gradient descent is very popular because it is simple and applicable to any differentiable function

#### How to Set Learning Rate $\alpha$ ?

 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

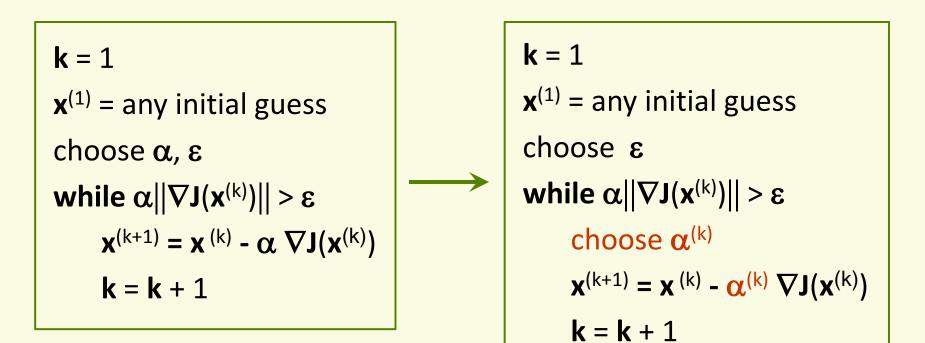
#### How to Set Learning Rate $\alpha$ ?

- 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  $\alpha$  at each iteration



## **Variable Learning Rate**

• Usually don't keep track of all intermediate solutions

```
k = 1

x^{(1)} = any initial guess

choose \alpha, \epsilon

while \alpha ||\nabla J(x^{(k)})|| > \epsilon

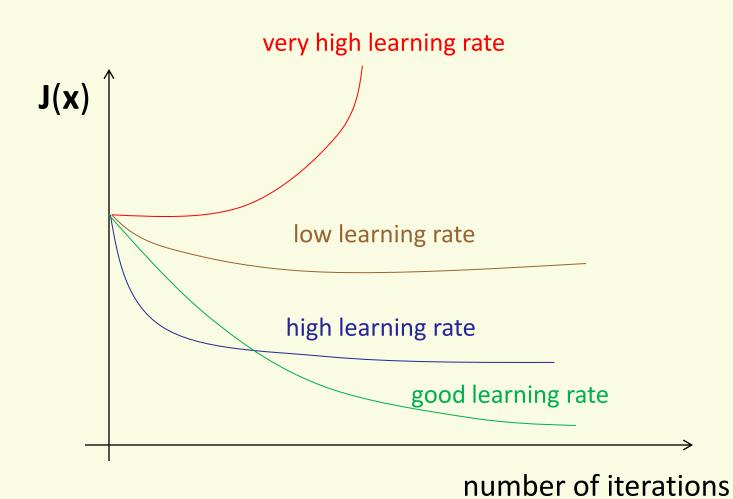
x^{(k+1)} = x^{(k)} - \alpha \nabla J(x^{(k)})

k = k + 1
```

**x** = any initial guess choose  $\alpha$ ,  $\varepsilon$ while  $\alpha ||\nabla J(x)|| > \varepsilon$  $x = x - \alpha \nabla J(x)$ 

## **Learning Rate**

 Monitor learning rate by looking at how fast the objective function decreases



### **Advanced Optimization Methods**

- There are more advanced gradient-based optimization methods
- Such as conjugate gradient
  - automatically pick a good learning rate  $\boldsymbol{\alpha}$
  - usually converge faster
  - however more complex to understand and implement
  - in Matlab, use **fminunc** for various advanced optimization methods

## **Supervised Learning Review**

• Training samples (or examples)

- Each example is typically multi-dimensional
  - $\mathbf{x}^{i} = [\mathbf{x}^{i}_{1}, \mathbf{x}^{i}_{2}, ..., \mathbf{x}^{i}_{d}]$
  - **x**<sup>i</sup> is often called a *feature vector*
- Know desired output for each example

- regression: continuous **y**
- classification: finite **y**

## **Supervised Learning Review**

- Wish to design a machine f(x,w) s.t.
   f(x,w) = y
  - How do we choose **f**?
    - last time studied kNN classifier
    - this lecture in on liner classifier
    - many other choices
  - **w** is multidimensional vector of weights (also called *parameters*)

$$w = [w_1, w_2, ..., w_k]$$

• By modifying **w**, the machine "learns"

## **Training and Testing Phases**

- Divide all labeled samples x<sup>1</sup>, x<sup>2</sup>,..., x<sup>n</sup> into training and test sets
- Training phase
  - Uses training samples
  - goal is to "teach" the machine
  - find weights w s.t. f(x<sup>i</sup>,w) = y<sup>i</sup> "as much as possible"
    - "as much as possible" needs to be defined
- Testing phase
  - Uses only test samples
  - for evaluating how well our machine works on unseen examples

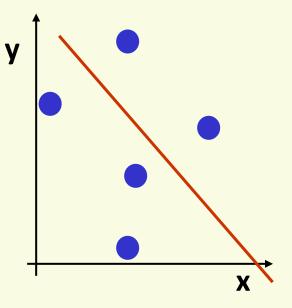
#### **Loss Function**

- How to quantify "**f**(**x**<sup>*i*</sup>,**w**) = **y**<sup>*i*</sup> as much as possible"?
- **f**(**x**,**w**) has to be "close" to the true output **y**
- Define Loss (or Error, or Criterion) function L
- First define per-sample loss L(x<sup>i</sup>,y<sup>i</sup>,w)
- Examples of loss function
  - for classification,  $L(x^i, y^i, w) = I[f(x^i, w) \neq y^i]$ 
    - I[true] = 1, I[false] = 0
  - for regression,  $\mathbf{L}(\mathbf{x}^{i},\mathbf{y}^{i},\mathbf{w}) = ||\mathbf{f}(\mathbf{x}^{i},\mathbf{w}) \mathbf{y}^{i}||^{2}$ ,
    - how far is the estimated output from the correct one?
- Then loss function  $\mathbf{L} = \Sigma_i \mathbf{L}(\mathbf{x}^i, \mathbf{y}^i, \mathbf{w})$ 
  - classification: counts number of misclassified examples
  - regression: sums distances to the correct output

### **Linear Machine: Regression**

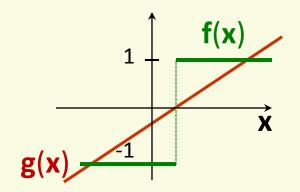
- $f(x,w) = w_0 + \sum_{i=1,2,...d} w_i x_i$
- In vector notation
  - $\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_d]$
  - $\mathbf{f}(\mathbf{x},\mathbf{w}) = \mathbf{w}_0 + \mathbf{w}^t \mathbf{x}$
- This is standard linear regression
  - line fitting
  - assume  $\mathbf{L}(\mathbf{x}^{i},\mathbf{y}^{i},\mathbf{w}) = ||\mathbf{f}(\mathbf{x}^{i},\mathbf{w}) \mathbf{y}^{i}||^{2}$
- optimal w can be found by solving a system of linear equations

$$\mathbf{w}^* = [\Sigma \mathbf{x}^i \ (\mathbf{x}^i)^T]^{-1} \Sigma \mathbf{y}^i \mathbf{x}^i$$

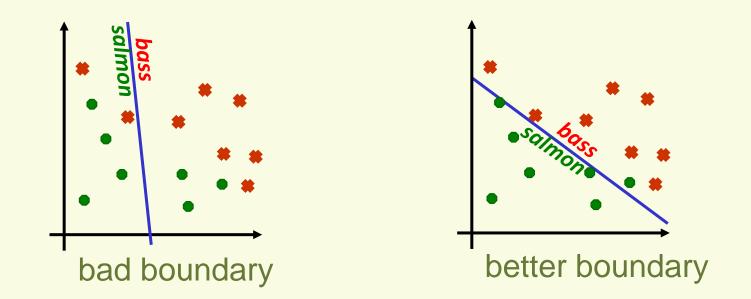


## **Linear Machine: Classification**

- First consider the two-class case
- Choose encoding
  - **y** = 1 for the first class
  - **y** = -1 for the second class
- Linear classifier
  - $-\infty \leq \mathbf{w}_0 + \mathbf{x}_1 \mathbf{w}_1 + \dots + \mathbf{x}_d \mathbf{w}_d \leq \infty$
  - we need f(x, w) to be either +1 or -1
  - let  $g(x,w) = w_0 + x_1 w_1 + ... + x_d w_d = w_0 + w^t x$
  - let f(x,w) = sign(g(x,w))
    - 1 if **g(x,w)** is positive
    - -1 if g(x,w) is negative
    - other choices for g(x,w) are also used
  - g(x,w) is called the discriminant function



#### **Linear Classifier: Decision Boundary**



- $\mathbf{f}(\mathbf{x},\mathbf{w}) = \operatorname{sign}(\mathbf{g}(\mathbf{x},\mathbf{w})) = \operatorname{sign}(\mathbf{w}_0 + \mathbf{x}_1\mathbf{w}_1 + \dots + \mathbf{x}_d\mathbf{w}_d)$
- Decision boundary is linear
- Find the best linear boundary to separate two classes
- Search for best  $\mathbf{w} = [\mathbf{w}_0, \mathbf{w}_1, \dots, \mathbf{w}_d]$  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  $\mathbf{g}(\mathbf{x}) = \mathbf{w}^{\mathsf{t}}\mathbf{x} + \mathbf{w}_{\mathsf{0}}$

decision boundary g(x) > 0 $\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{0}$ **X**<sub>2</sub> decision region for class 1 g(x) < 0**X**<sub>1</sub> decision region for class 2

weight vector bias or threshold

#### **More on Linear Discriminant Function (LDF)**

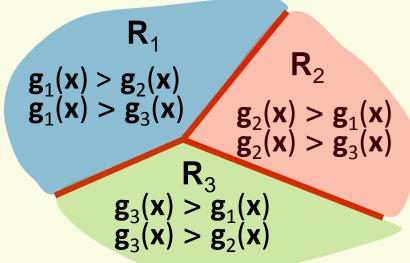
- Decision boundary:  $\mathbf{g}(\mathbf{x},\mathbf{w}) = \mathbf{w}_0 + \mathbf{x}_1 \mathbf{w}_1 + \dots + \mathbf{x}_d \mathbf{w}_d = 0$
- This is a hyperplane, by definition
  - a point in 1D
  - a line in 2D
  - a plane in 3D
  - a hyperplane in higher dimensions

## **Multiple Classes**

- 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

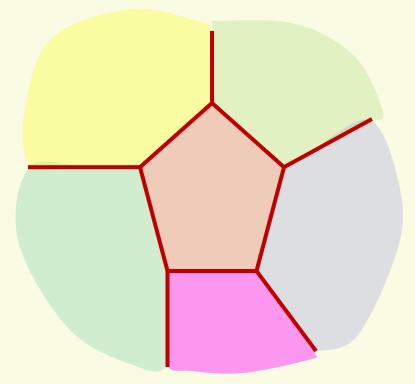
 $\mathbf{g}_{i}(\mathbf{x}) > \mathbf{g}_{j}(\mathbf{x})$  for all  $\mathbf{j} \neq \mathbf{i}$ 

- Let **R**<sub>i</sub> be the decision region for class **i** 
  - all examples in R<sub>i</sub> get assigned class i



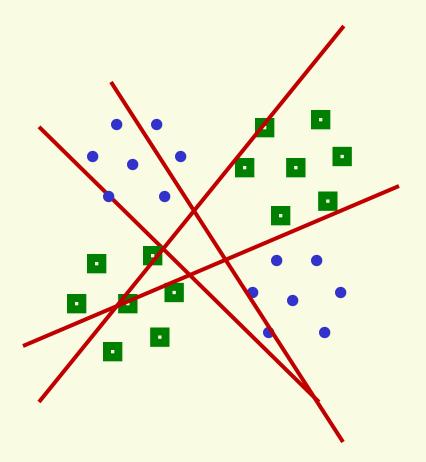
## **Multiple Classes**

- 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



## **Linear Classifiers**

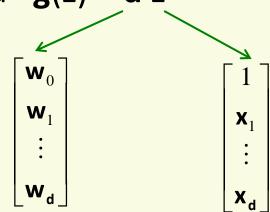
- Give simple decision boundary
  - try simpler models first
  - can still overfit in very high dimensions
- Optimal for certain type of data
  - Gaussian distributions with equal covariance
- May not be optimal for other data distributions, but they are very simple to use

#### **Fitting Parameters w**

- Linear discriminant function g(x) = w<sup>t</sup>x + w<sub>0</sub>
- Can rewrite it  $\mathbf{g}(\mathbf{x}) = \begin{bmatrix} \mathbf{w}_0 & \mathbf{w}^T \\ \mathbf{w}_0 & \mathbf{w}^T \end{bmatrix} \begin{bmatrix} 1 \\ \mathbf{x} \\ \mathbf{x} \end{bmatrix} = \mathbf{a}^T \mathbf{z} = \mathbf{g}(\mathbf{z})$

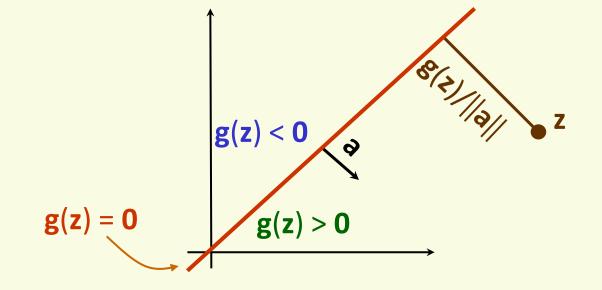
feature vector **z** 

- z is called augmented feature vector
- new problem equivalent to the old  $g(z) = a^{t}z$



#### **Augmented Feature Vector**

- Feature augmenting is done to simplify notation
- The rest of this lecture assumes augmented features
  - given samples x<sup>1</sup>,..., x<sup>n</sup> convert them to augmented samples z<sup>1</sup>,..., z<sup>n</sup> by adding a new dimension of value 1
- g(z) = a<sup>t</sup>z



## **Training Error**

- Assume we have 2 classes
- Samples z<sup>1</sup>,..., z<sup>n</sup> some in class 1, some in class 2
- Use samples to determine weights a in g(z) = a<sup>t</sup>z
- Want to minimize number of misclassified samples

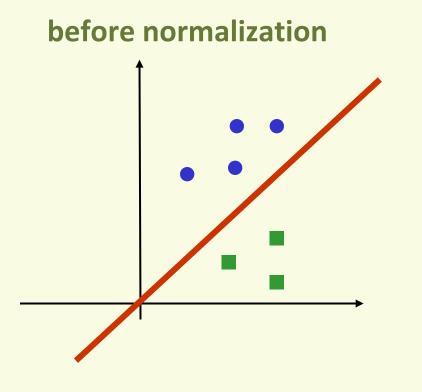
• Recall that 
$$\begin{cases} g(\mathbf{z}^i) > 0 \implies \text{class 1} \\ g(\mathbf{z}^i) < 0 \implies \text{class 2} \end{cases}$$

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

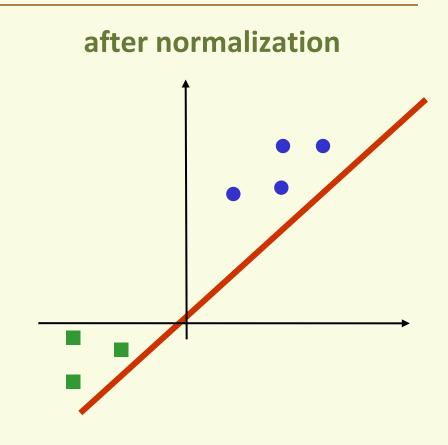
## **Simplifying Notation Further**

- Thus training error is 0 if  $\begin{cases} a^{t}z^{i} > 0 & \forall z^{i} \text{ class } 1 \\ a^{t}z^{i} < 0 & \forall z^{i} \text{ class } 2 \end{cases}$
- Equivalently, training error is 0 if  $\begin{cases} a^{t}z^{i} > 0 \ \forall z^{i} \text{ class 1} \\ a^{t}(-z^{i}) > 0 \ \forall z^{i} \text{ class 2} \end{cases}$
- Problem "normalization":
  - 1. replace all examples  $z^i$  from class 2 by  $-z^i$
  - 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 **x**<sup>1</sup>,... **x**<sup>n</sup> can also be linearly separated

## **Effect of Normalization**



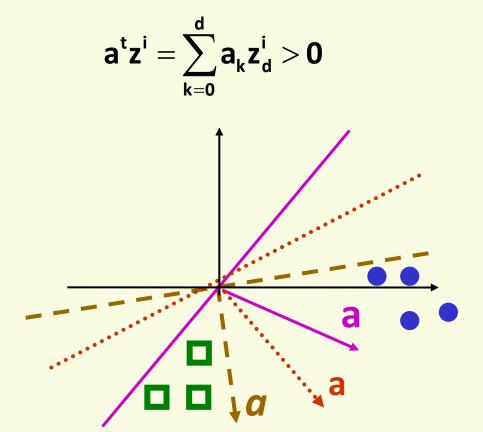
seek a hyperplane that separates samples from different categories



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

### **Solution Region**

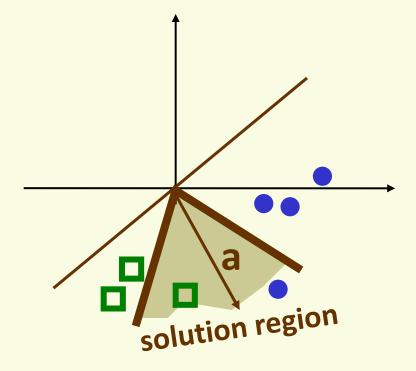
• Find weight vector **a** s.t. for all samples **z**<sup>1</sup>,...,**z**<sup>n</sup>



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

### **Solution Region**

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



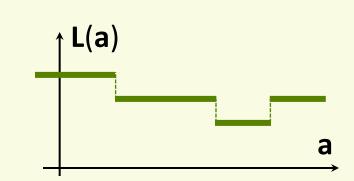
#### **Design a Loss Function**

- Find weight vector **a** s.t.  $\forall z^1,..., z^n$ ,  $a^t z^i > 0$
- Design a loss function L(a), which is minimum when a is a solution vector
- Let Z(a) be the set of examples misclassified by a
   Z(a) = { z<sup>i</sup> | a<sup>t</sup> z<sup>i</sup> < 0 }</li>

• Natural choice: number of misclassified examples

L(a) = |Z(a)|

- Unfortunately, cannot minimize with gradient descent
  - piecewise constant, gradient zero or does not exist

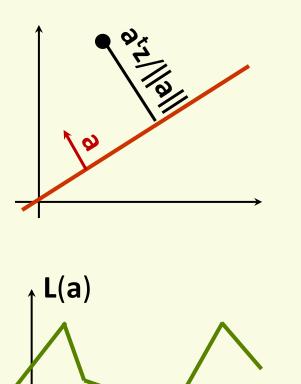


## **Perceptron Loss Function**

Better choice: Perceptron loss function

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

- If z is misclassified, a<sup>t</sup>z < 0</li>
- Thus L(a) ≥ 0
- L<sub>p</sub>(a) is proportional to the sum of distances of misclassified examples to decision boundary
- L<sub>p</sub>(a) is piecewise linear and suitable for gradient descent



### **Optimizing with Gradient Descent**

$$\mathbf{L}_{\mathbf{p}}(\mathbf{a}) = \sum_{\mathbf{z} \in \mathbf{Z}(\mathbf{a})} \left( - \mathbf{a}^{\mathsf{t}} \mathbf{z} \right)$$

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

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

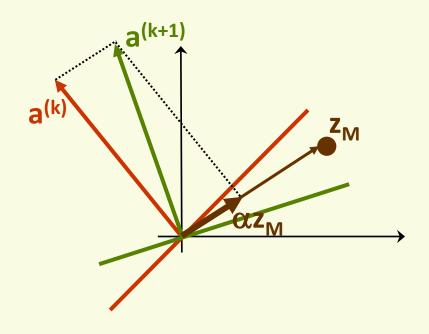
• Gradient decent update rule for  $L_p(a)$  is:

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

• called **batch rule** because it is based on all examples

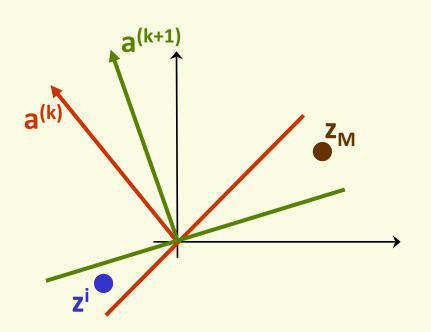
## **Perceptron Single Sample Rule**

- Gradient decent single sample rule for  $L_p(a)$  is  $a^{(k+1)} = a^{(k)} + \alpha \cdot z_M$ 
  - **z<sub>M</sub>** is one sample misclassified by **a**<sup>(k)</sup>
  - must have a consistent way to visit samples
- Geometric Interpretation:
- $\mathbf{z}_{\mathbf{M}}$  misclassified by  $\mathbf{a}^{(k)}$  $\left(\mathbf{a}^{(k)}\right)^{t} \mathbf{z}_{\mathbf{M}} \leq \mathbf{0}$
- z<sub>M</sub> is on the wrong side of decision boundary
- adding α·z<sub>M</sub> to a moves decision boundary in the right direction

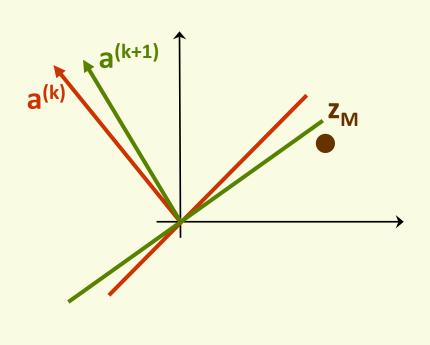


### **Perceptron Single Sample Rule**

if α is too large, previously correctly classified sample **z**<sup>i</sup> is now misclassified



if  $\pmb{\alpha}$  is too small,  $\, \pmb{z}_{M}^{}$  is still misclassified



## **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  $\mathbf{k} \rightarrow \infty$
    - 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

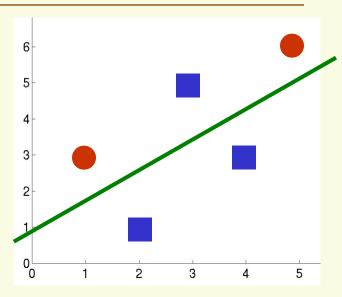
- True gradient descent, full gradient computed
- Smoother gradient because all samples are used
- Takes longer to converge

### 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

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

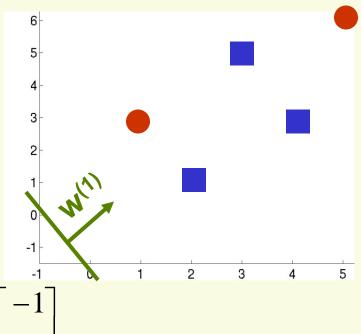
$$\mathbf{z}^{1} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} \qquad \mathbf{z}^{2} = \begin{bmatrix} 1 \\ 4 \\ 3 \end{bmatrix} \qquad \mathbf{z}^{3} = \begin{bmatrix} 1 \\ 3 \\ 5 \end{bmatrix} \qquad \mathbf{z}^{4} = \begin{bmatrix} -1 \\ -1 \\ -3 \end{bmatrix} \qquad \mathbf{z}^{5} = \begin{bmatrix}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



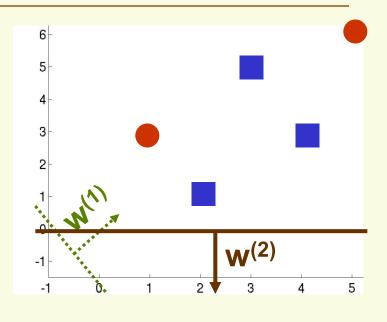
- single sample perceptron rule
- Initial weights **a**<sup>(1)</sup> = [1 1 1]
- This is line  $\mathbf{x}_1 + \mathbf{x}_2 + 1 = 0$
- Use fixed learning rate  $\alpha = 1$
- Rule is:  $a^{(k+1)} = a^{(k)} + z_{M}$

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

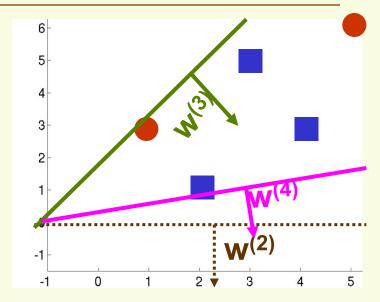
- $\mathbf{a}^{\mathsf{t}}\mathbf{z}^{\mathsf{1}} = [1 \ 1 \ 1] \cdot [1 \ 2 \ 1]^{t} > 0$
- $\mathbf{a}^{\mathsf{t}}\mathbf{z}^2 = [1\ 1\ 1] \cdot [1\ 4\ 3]^t > 0$
- $\mathbf{a}^{\mathsf{t}}\mathbf{z}^{\mathsf{3}} = [1\ 1\ 1] \cdot [1\ 3\ 5]^{\mathsf{t}} > 0$



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

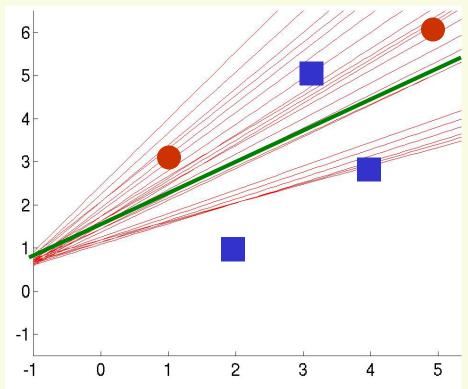


- $\mathbf{a}^{(3)} = [1 \ 2 \ -1]$
- rule is: a<sup>(k+1)</sup> = a<sup>(k)</sup> + z<sub>M</sub>
  - $\mathbf{z}^{1} = \begin{bmatrix} \mathbf{1} \\ \mathbf{2} \\ \mathbf{1} \end{bmatrix} \mathbf{z}^{2} = \begin{bmatrix} 1 \\ 4 \\ 3 \end{bmatrix} \mathbf{z}^{3} = \begin{bmatrix} 1 \\ 3 \\ 5 \end{bmatrix} \mathbf{z}^{4} = \begin{bmatrix} -1 \\ -1 \\ -3 \end{bmatrix} \mathbf{z}^{5} = \begin{bmatrix} -1 \\ -5 \\ -6 \end{bmatrix}$



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

- Can continue this forever
  - there is no solution vector a satisfying for all a<sup>t</sup>z<sub>i</sub> > 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?

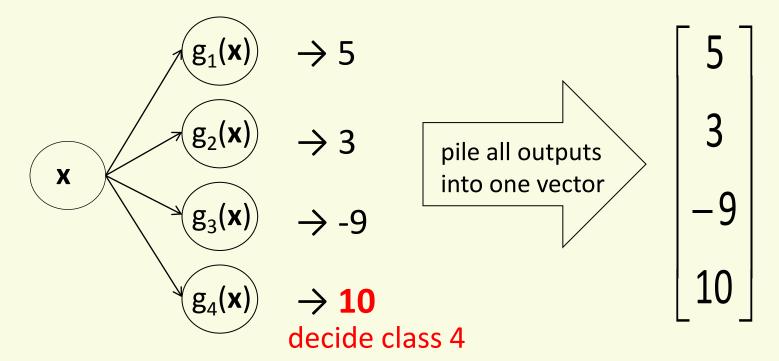


#### **Linear Classifier: Multiple Classes**

- Can extend to **m** class case
- Augment samples with 1 as the first feature
  - but no "normalization"
- Define **m** discriminant functions

$$g_i(x) = w_i^t x$$
 for  $i = 1, 2, ... m$ 

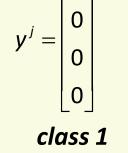
Assign x to i that gives maximum g<sub>i</sub>(x)



### **Linear Classifier: Multiple Classes**

- Could use one dimensional output  $y_i \in \{1, 2, 3, ..., m\}$
- Convenient to use multi-dimensional outputs

 $y^{j} = \begin{vmatrix} 1 \\ 0 \end{vmatrix}$ 



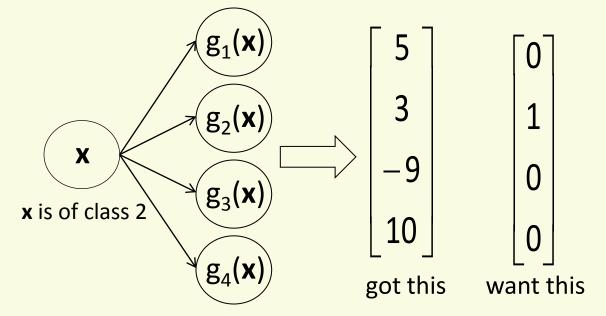
class 2



 $y^{j} = \begin{vmatrix} 0 \\ 1 \end{vmatrix}$ 



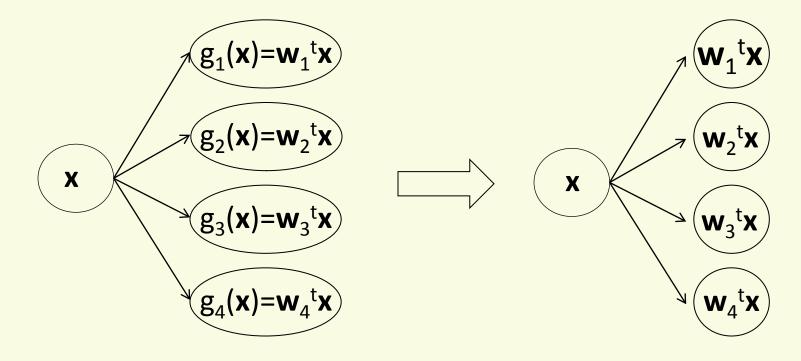
 For training, if sample is of class i, want output vector to be 0 everywhere except position i, where it should be 1



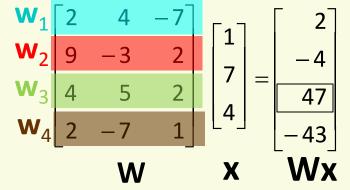
 $y^{j} =$ 

#### **Linear Classifier: Multiple Classes**

Assign x to i that gives maximum g<sub>i</sub>(x) = w<sub>i</sub><sup>t</sup>x



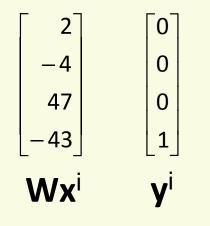
• In matrix notation



Assign x to class that corresponds to largest row of Wx

#### **Linear Multiclass Classifier: Loss Function**

- Assign sample x<sup>i</sup> to class that corresponds to largest row of Wx<sup>i</sup>
- Loss function?



- Can use quadratic loss per sample  $\mathbf{x}^{i}$  as  $\frac{1}{2} \|\mathbf{W}\mathbf{x}^{i} \mathbf{y}^{i}\|^{2}$ 
  - for example above, loss  $(2^2 + 4^2 + 47^2 + 44^2)/2$
  - total loss on all training samples  $L(\mathbf{W}) = \frac{1}{2} \Sigma_i || \mathbf{W} \mathbf{x}^i \mathbf{y}^i ||^2$
  - gradient of the loss

$$\nabla \mathbf{L}(\mathbf{W}) = \sum_{i} (\mathbf{W} \mathbf{x}^{i} - \mathbf{y}^{i}) (\mathbf{x}^{i})^{t}$$

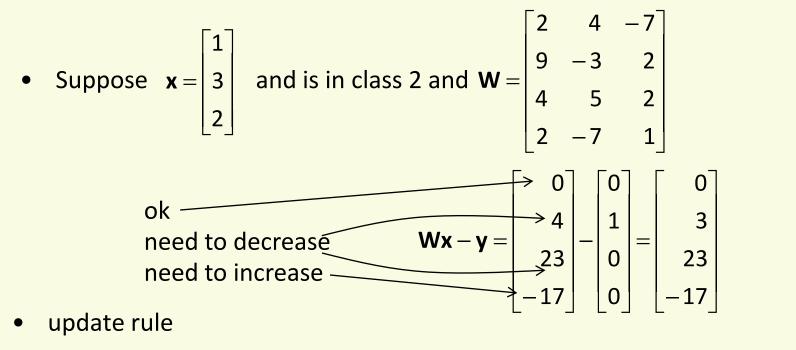
• batch gradient descent updates

$$\mathbf{W} = \mathbf{W} - \alpha \sum_{i} \left( \mathbf{W} \mathbf{x}^{i} - \mathbf{y}^{i} \right) \left( \mathbf{x}^{i} \right)^{t}$$

#### Linear Multiclass: Quadratic Loss

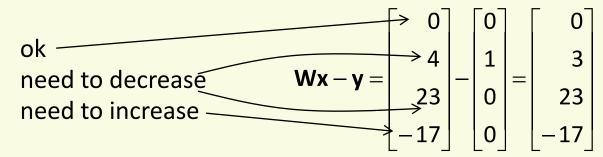
• Consider gradient descent update, single sample **x** with  $\alpha = 1$ 

$$W = W - (Wx - y)x^{t}$$



$$\mathbf{W} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 3 \\ 23 \\ -17 \end{bmatrix} \begin{bmatrix} 1 & 3 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} - \begin{bmatrix} 0 \cdot (1 & 2 & 3) \\ 3 \cdot (1 & 2 & 3) \\ 23 \cdot (1 & 2 & 3) \\ -17 \cdot (1 & 2 & 3) \end{bmatrix}$$

#### **Linear Multiclass: Quadratic Loss**



• update rule

$$\mathbf{W} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 3 \\ 23 \\ -17 \end{bmatrix} \begin{bmatrix} 1 & 3 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} - \begin{bmatrix} 0 \cdot (1 & 2 & 3) \\ 3 \cdot (1 & 2 & 3) \\ 23 \cdot (1 & 2 & 3) \\ -17 \cdot (1 & 2 & 3) \end{bmatrix} = \begin{bmatrix} 2 & 4 & -7 \\ 6 & -12 & -4 \\ -19 & -64 & -44 \\ 19 & 44 & 35 \end{bmatrix}$$

• With new W

$$\mathbf{W}\mathbf{x} = \begin{bmatrix} 0\\ -38\\ -299\\ 221 \end{bmatrix}$$

#### **Linear Multiclass: Perceptron Loss Function**

- Assign sample x<sup>i</sup> to class that corresponds to largest row of Wx<sup>i</sup>
- Another loss function?

$$\begin{bmatrix}
2 \\
-4 \\
0 \\
47 \\
-43
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
1
\end{bmatrix}$$

- Perceptron loss on sample  $\mathbf{x}^i$ :  $\mathbf{L}_i(\mathbf{W}) = \max_{\mathbf{k}}[(\mathbf{W}\mathbf{x}^i)_k (\mathbf{W}\mathbf{x}^i)_c]$ , where
  - (**Wx**<sup>i</sup>)<sub>k</sub> is the entry in row **k** of vector **Wx**<sup>i</sup>
  - **c** is the correct class of sample **x**<sup>i</sup>
  - in words, find the largest entry in Wx<sup>i</sup>, subtract from it the entry in the row corresponding to the true class of sample x<sup>i</sup>
    - loss is zero if correct classification, positive otherwise
  - for the example above, loss is 47-(-43)= 90 since sample is of class 4

#### **Linear Multiclass: Perceptron Loss Function**

- $\mathbf{L}_{i}(\mathbf{W}) = \max_{\mathbf{k}} [(\mathbf{W}\mathbf{x}^{i})_{\mathbf{k}} (\mathbf{W}\mathbf{x}^{i})_{\mathbf{c}}]$
- Gradient, single sample rule
  - let c be the correct row, and r be row where Wx<sup>i</sup> gives the largest output

• if 
$$\mathbf{r} = \mathbf{c}$$
,  $\nabla \mathbf{L}_{\mathbf{i}}(\mathbf{W}) = \mathbf{0}$ 

$$\mathbf{x}^{i} = \begin{bmatrix} 1\\3\\2 \end{bmatrix} \begin{bmatrix} 2\\-4\\47\\-43 \end{bmatrix} \begin{bmatrix} 0\\0\\0\\1 \end{bmatrix}$$

• otherwise, 
$$\nabla \mathbf{L}_{i}(\mathbf{W}) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \mathbf{X}^{i} & \mathbf{V} \\ 0 & 0 & 0 & 0 \\ \mathbf{-X}^{i} & \mathbf{V} \end{bmatrix}$$
 row **r**  
• for the example,  $\nabla \mathbf{L}_{i}(\mathbf{W}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 3 & 2 \\ -1 & -3 & -2 \end{bmatrix}$ 

#### **Linear Multiclass: Perceptron Loss Function**

• For the example,

$$\nabla \mathbf{L}_{\mathbf{i}}(\mathbf{W}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 3 & 2 \\ -1 & -3 & -2 \end{bmatrix} \qquad \mathbf{x}^{\mathbf{i}} = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$
$$\mathbf{y}^{\mathbf{i}}$$
$$\mathbf{y}^{\mathbf{i}}$$

With 
$$\alpha = 1$$
, new  $\mathbf{W} = \begin{bmatrix} 2 & 1 & 1 & 1 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 \\ 1 & 3 & 2 \\ -1 & -3 & -2 \end{bmatrix} = \begin{bmatrix} 9 \\ 9 \\ 3 \\ 3 \end{bmatrix}$ 

**□** 

• With new weights:

$$\mathbf{W}\mathbf{x}^{\mathbf{i}} = \begin{bmatrix} \mathbf{0} \\ \mathbf{4} \\ \mathbf{9} \\ -\mathbf{3} \end{bmatrix}$$

• Compare to the old weights:

$$\mathbf{W}_{\mathsf{old}}\mathbf{x}^{\mathsf{i}} = \begin{bmatrix} 0\\ 4\\ 23\\ -17 \end{bmatrix}$$

3

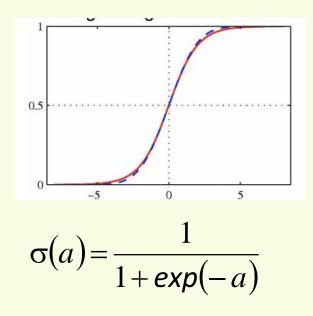
-4

#### **Three Approaches to Classification**

- 1. Directly design discriminant function **f**(**x**,**w**) for classification
  - design differentiable loss function that makes intuitive sense
  - find **w** that minimize loss function
  - Choose class that maximizes discriminant function
- 2. Model conditional class probabilities P(class=k|x,w)
  - Choose loss function with probabilistic interpretation and minimize it
    - Loss function is usually (–log probability)
    - Parameters w are tuned so as to maximize probability of the training data
  - Choose class that maximizes discriminant function
- 3. Model probability of training data **x** under class-specific generative models p(**x**,**w**)
  - Use training data to fit parameters **w** for each class independently
    - i.e. fit Gaussians to samples from each class
  - Choose the class that makes **x** most probable

## Linear Machine: Logistic Regression

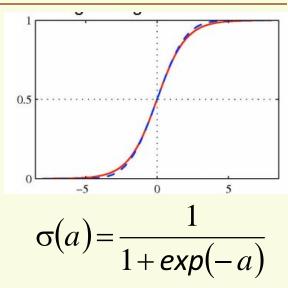
- Has probabilistic interpretation
- Model P(class 1|x,w) and P(class 2|x,w)
- Uses logistic sigmoid function
  - denote classes with 1 and 0 now
    - **y**<sup>i</sup> = 1 for class 1, **y**<sup>i</sup> = 0 for class 2
- $g(x,w) = w^T x$
- let  $\mathbf{f}(\mathbf{x},\mathbf{w}) = \mathcal{O}(\mathbf{g}(\mathbf{x},\mathbf{w})) = \mathcal{O}(\mathbf{w}^{\mathsf{T}}\mathbf{x})$ 
  - assume **x** is augmented with 1
  - bigger 0.5 if **w<sup>T</sup>x** is positive, decide class 1
  - less 0.5 if **w<sup>T</sup>x** is negative, decide class 2
- Probabilistic interpretation
  - $P(class 1|x,w) = G(w^Tx)$
  - **P**(class 2 | **x**, **w**) = 1 P(class 1 | **x**, **w**)
- Despite the name, logistic regression is used for classification, not regression
  - Side note: sigmoid is a continuous function, good for gradient descent



# **Linear Machine: Logistic Regression**

- $f(x,w) = G(w^T x)$
- Probabilistic interpretation
  - $P(class 1|x,w) = G(w^Tx)$
  - **P**(class 2 | **x**, **w**) = 1 **P**(class 1 | **x**, **w**)
- Per sample loss function: -log( P( y<sup>i</sup> | x<sup>i</sup>) )
  - if sample x<sup>i</sup> of class 1, loss is -log(σ(w<sup>T</sup>x<sup>i</sup>))
  - if sample x<sup>i</sup> of class 2, loss is -log(1-σ(w<sup>T</sup>x<sup>i</sup>))
- Convex, can be optimized exactly with gradient descent
- Gradient descent update rule

$$\boldsymbol{w} = \boldsymbol{w} + \alpha \sum_{j} \left( \boldsymbol{y}^{j} - \boldsymbol{\sigma} \left( \boldsymbol{w}^{t} \boldsymbol{x}^{j} \right) \right) \boldsymbol{x}^{j}$$

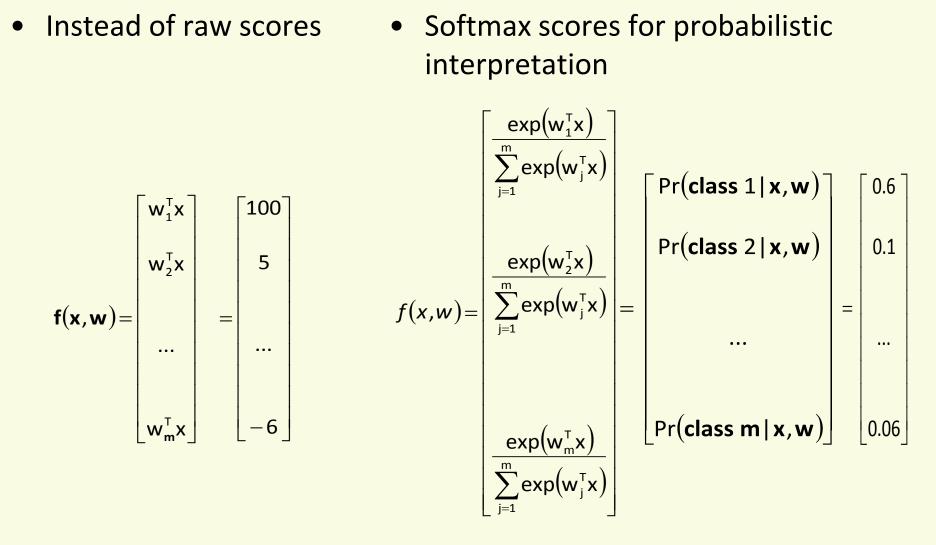


# **Linear Machine: Softmax Regression**

In case of **m** classes, define **m** functions

$$g_i(x) = w_i^t x$$
 for  $i = 1, 2, ... m$ 

- Instead of raw scores
- Softmax scores for probabilistic



## **Linear Machine: Softmax Regression**

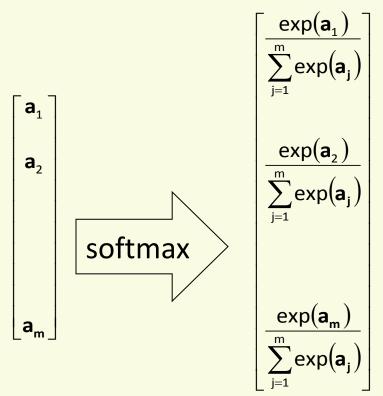
• Also optimize under -log( Pr( y<sup>i</sup> | x<sup>i</sup>) ) loss function

$$f(x,w) = \begin{bmatrix} \frac{\exp(w_1^{\mathsf{T}}x)}{\sum_{j=1}^{m} \exp(w_j^{\mathsf{T}}x)} \\ \frac{\exp(w_2^{\mathsf{T}}x)}{\sum_{j=1}^{m} \exp(w_j^{\mathsf{T}}x)} \\ \frac{\exp(w_1^{\mathsf{T}}x)}{\sum_{j=1}^{m} \exp(w_j^{\mathsf{T}}x)} \end{bmatrix} = \begin{bmatrix} \Pr(\operatorname{class} 1 | x, w) \\ \Pr(\operatorname{class} 2 | x, w) \\ \dots \\ \Pr(\operatorname{class} 2 | x, w) \\ \dots \\ \Pr(\operatorname{class} m | x, w) \end{bmatrix} \begin{pmatrix} 0.6 \\ 0.1 \\ \dots \\ 0.06 \end{bmatrix}$$
  
if sample of class 2, take -log of the number in row 2 for

the loss

## **Linear Machine: Softmax Regression**

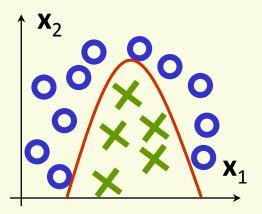
• Define softmax(**a**) function for vector **a** as



Update rule for weight matrix W

$$\mathbf{W} = \mathbf{W} + \alpha \sum_{j} \left( \mathbf{y}^{j} - \sigma \left( \mathbf{w}^{\mathsf{T}} \mathbf{x}^{j} \right) \right) \left( \mathbf{x}^{j} \right)^{\mathsf{t}}$$

 Can use other discriminant functions, like quadratics g(x) = w<sub>0</sub>+w<sub>1</sub>x<sub>1</sub>+w<sub>2</sub>x<sub>2</sub>+ w<sub>12</sub>x<sub>1</sub>x<sub>2</sub> +w<sub>11</sub>x<sub>1</sub><sup>2</sup> +w<sub>22</sub>x<sub>2</sub><sup>2</sup>



- Methodology is almost the same as in the linear case
  - $\mathbf{f}(\mathbf{x}) = \operatorname{sign}(\mathbf{w}_0 + \mathbf{w}_1 \mathbf{x}_1 + \mathbf{w}_2 \mathbf{x}_2 + \mathbf{w}_{12} \mathbf{x}_1 \mathbf{x}_2 + \mathbf{w}_{11} \mathbf{x}_1^2 + \mathbf{w}_{22} \mathbf{x}_2^2)$

| • | <b>z</b> = | [1 | $\mathbf{X}_{1}$ | <b>X</b> <sub>2</sub> | $\mathbf{X}_1 \mathbf{X}_2$ | <b>x</b> <sub>1</sub> <sup>2</sup> | <b>x</b> <sub>2</sub> <sup>2</sup> ] |
|---|------------|----|------------------|-----------------------|-----------------------------|------------------------------------|--------------------------------------|
|   |            | г  |                  |                       |                             |                                    | ٦                                    |

- **a** =  $[\mathbf{w}_0 \ \mathbf{w}_1 \ \mathbf{w}_2 \ \mathbf{w}_{12} \ \mathbf{w}_{11} \ \mathbf{w}_{22}]$
- "normalization": multiply negative class samples by -1
- all the other procedures remain the same, i.e. gradient descent to minimize Perceptron loss function, any other loss function

• In general, to the liner function:

$$\mathbf{g}(\mathbf{x},\mathbf{w}) = \mathbf{w}_0 + \sum_{i=1...d} \mathbf{w}_i \mathbf{x}_i$$

• can add quadratic terms:

$$\mathbf{g}(\mathbf{x},\mathbf{w}) = \mathbf{w}_0 + \sum_{i=1...d} \mathbf{w}_i \mathbf{x}_i + \sum_{i=1...d} \sum_{j=1,...d} \mathbf{w}_{ij} \mathbf{x}_i \mathbf{x}_j$$

- This is still a linear function in its parameters w
- $\mathbf{g}(\mathbf{y},\mathbf{v}) = \mathbf{v}_0 + \mathbf{v}^t \mathbf{y}$

 $\mathbf{v}_{0} = \mathbf{w}_{0}$  $\mathbf{y} = [\mathbf{x}_{1} \ \mathbf{x}_{2} \dots \ \mathbf{x}_{d} \ \mathbf{x}_{1} \mathbf{x}_{1} \ \mathbf{x}_{1} \mathbf{x}_{2} \ \dots \ \mathbf{x}_{d} \mathbf{x}_{d}]$  $\mathbf{v} = [\mathbf{w}_{1} \ \mathbf{w}_{2} \dots \ \mathbf{w}_{d} \ \mathbf{w}_{11} \ \mathbf{w}_{12} \ \dots \ \mathbf{w}_{dd}]$ 

• Can use all the same training methods as before

• Generalized linear classifier

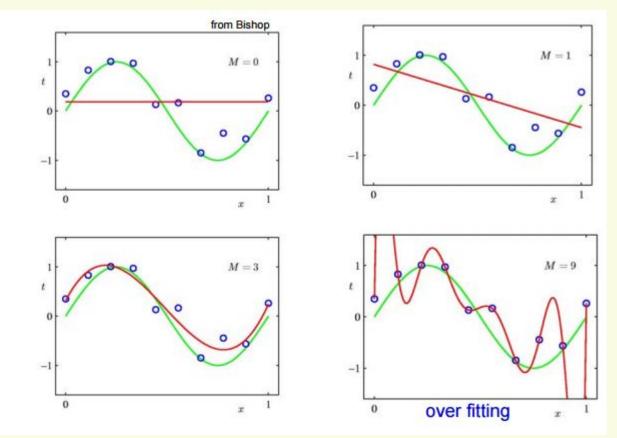
$$\mathbf{g}(\mathbf{x},\mathbf{w}) = \mathbf{w}_0 + \sum_{i=1...m} \mathbf{w}_i \mathbf{h}_i(\mathbf{x})$$

- h(x) are called basis function, can be arbitrary functions
  - in strictly linear case, h<sub>i</sub>(x) = x<sub>i</sub>
- Linear function in its parameters **w**

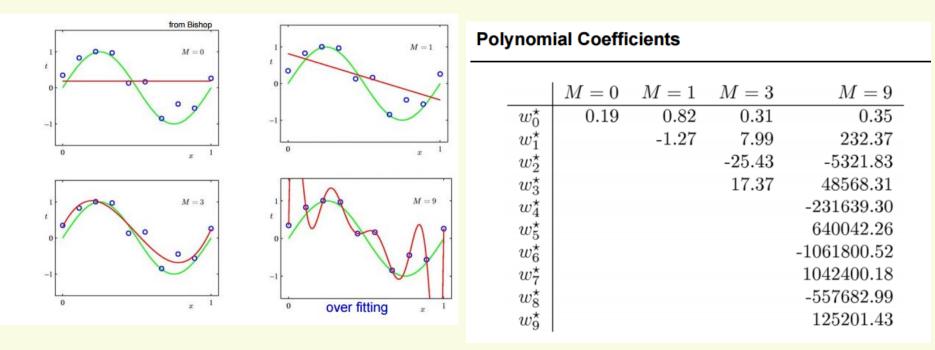
$$g(x,w) = w_0 + w^t h$$
  
 $h = [h_1(x) h_2(x) \dots h_m(x)]$   
 $[w_1 \dots w_m]$ 

• Can use all the same training methods as before

- Usually face severe overfitting
  - too many degrees of freedom
  - boundary can "curve" to fit to the noise in the data
- Regression example



- Helps to regularize by keeping w small
  - small **w** means the boundary is not as curvy
- Regression example



- Helps to *regularize* by keeping **w** small
  - small **w** means the boundary is not as curvy
- For example, add  $\lambda ||w||^2$  to the loss function
- Recall quadratic loss function

$$L = \frac{1}{2} \sum_{i} || \mathbf{f}(\mathbf{x}^{i}, \mathbf{w}) - \mathbf{y}^{i} ||^{2}$$

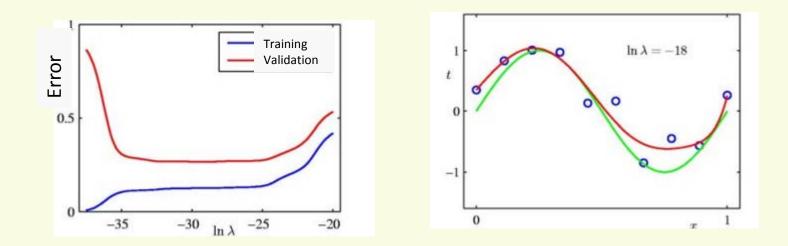
Regularized version

$$L = \frac{1}{2} \Sigma_i || f(x^i, w) - y^i ||^2 + \lambda ||w||^2$$

 Regression example, polynomial coefficients for degree M = 9

|               | $\ln\lambda=-\infty$ | $\ln\lambda=-18$ | $\ln\lambda=0$ |
|---------------|----------------------|------------------|----------------|
| $w_0^\star$   | 0.35                 | 0.35             | 0.13           |
| $w_1^\star$   | 232.37               | 4.74             | -0.05          |
| $w_2^\star$   | -5321.83             | -0.77            | -0.06          |
| $w_3^\star$   | 48568.31             | -31.97           | -0.05          |
| $w_4^{\star}$ | -231639.30           | -3.89            | -0.03          |
| $w_5^{\star}$ | 640042.26            | 55.28            | -0.02          |
| $w_6^\star$   | -1061800.52          | 41.32            | -0.01          |
| $w_7^{\star}$ | 1042400.18           | -45.95           | -0.00          |
| $w_8^\star$   | -557682.99           | -91.53           | 0.00           |
| $w_9^{\star}$ | 125201.43            | 72.68            | 0.01           |

- How to set  $\lambda$ ?
- With validation or cross-validation
- Consider polynomial of degree M=9 regression



## **Learning by Gradient Descent**

- Can have classifiers even more general than generalized linear
- Suppose we suspect that the machine has to have functional form **f**(**x**,**w**), not necessarily linear
- Pick differentiable per-sample loss function **L**(**x**<sup>*i*</sup>, **y**<sup>*i*</sup>, **w**)
- Need to find w that minimizes  $\mathbf{L} = \Sigma_i \mathbf{L}(\mathbf{x}^i, \mathbf{y}^i, \mathbf{w})$
- Use gradient-based minimization:
  - Batch rule:  $\mathbf{w} = \mathbf{w} \alpha \nabla \mathbf{L}(\mathbf{w})$
  - Or single sample rule: W = W  $\alpha \nabla L(\mathbf{x}^{i}, \mathbf{y}^{i}, \mathbf{w})$