

CS4442/9542b
Artificial Intelligence II
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Lecture 5

Machine Learning

Linear Classifier

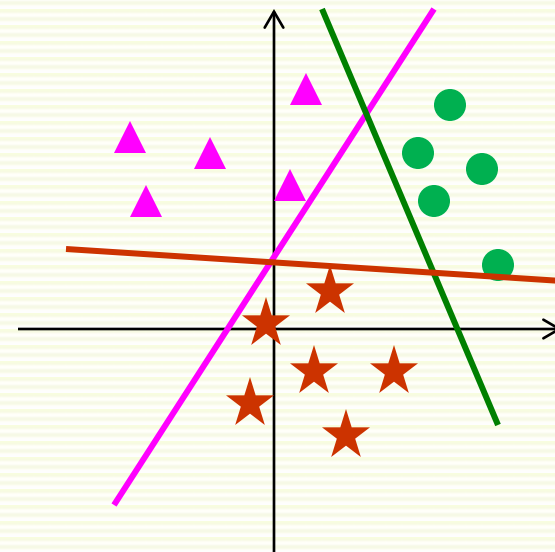
Multiple Classes

Outline

- Linear Classifier
 - Multiple classes
 1. Use collection of 2-class classifiers
 - one vs. all
 - all pairs
 2. Design multi-class loss functions
 - Perceptron Loss Function
 - Softmax Loss Function
 - Weight Regularization

Using 2-class Case: One vs. All

- Have classes 1, 2, ... , **m**
- Can construct multi-class classifier based on 2-class classifiers
- One way
 - Assume each 2-class classifier also gives confidence
 - Distance from separating hyperplane
 - Higher distance, more confidence
 - Train **m** 2-class classifiers
 - **1** vs other classes
 - **2** vs. other classes
 -
 - **m** vs. other classes
 - Make sure number of examples is balanced during training
 - At test time, run new sample through **m** binary classifiers
 - highest confidence class “wins”
- Works for any type of 2-class classifier, not just linear



Using 2-class Case: All pairs

- Train 2-class classifier for each distinct pair of classes (i,j)

	1	2	3	4
1		✓	✓	✓
2			✓	✓
3				✓
4				

- At test time, run new example \mathbf{x} through all binary classifiers
 - Choose most frequently occurring class
 - For example, \mathbf{x} was classified
 - 1 time as class 1
 - 2 times as class 2
 - 0 times as class 3
 - 3 times as class 4

} decide class 4

Multiple Classes: General Case

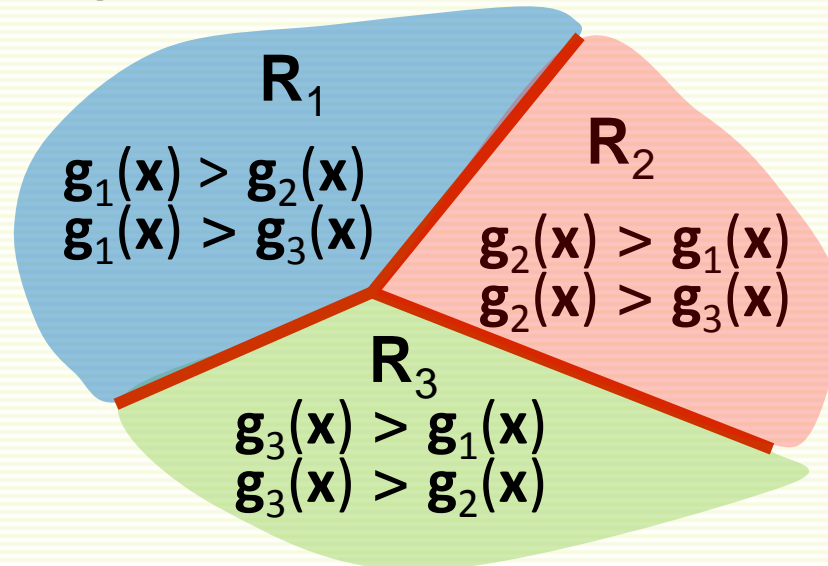
- General multiclass case
 - not based on 2-class classifiers
- Define m linear discriminant functions

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

- Assign \mathbf{x} to class i if

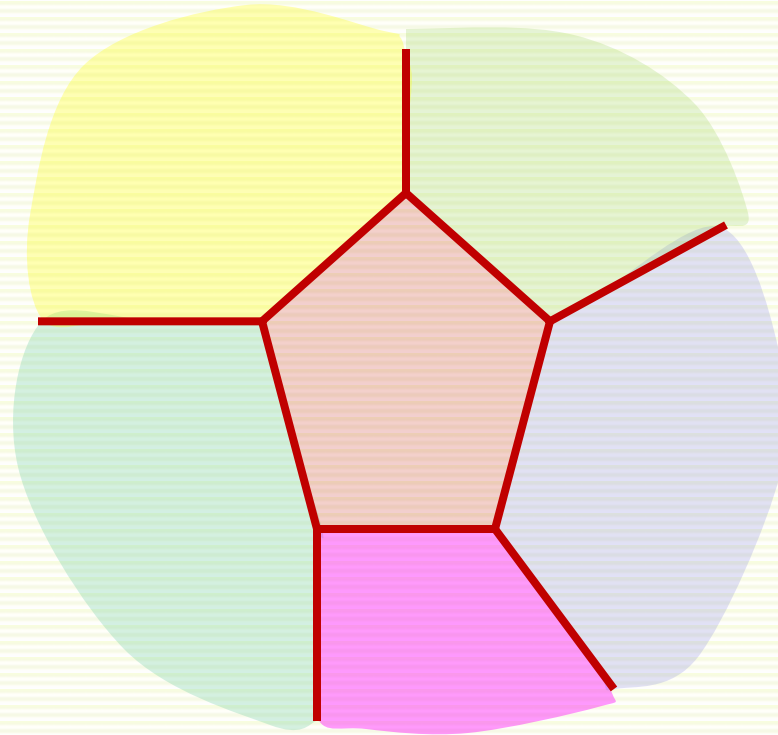
$$\mathbf{g}_i(\mathbf{x}) > \mathbf{g}_j(\mathbf{x}) \quad \text{for all } j \neq i$$

- Let R_i be decision region for class i
 - all samples in R_i assigned to class i



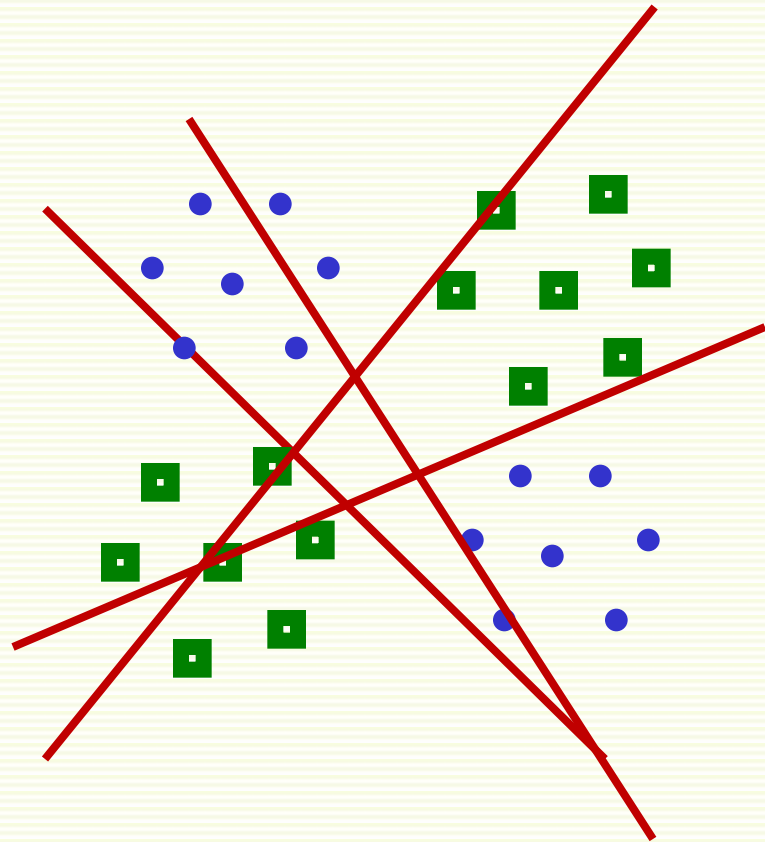
Multiple Classes

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



Failure Case for Linear Classifier

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

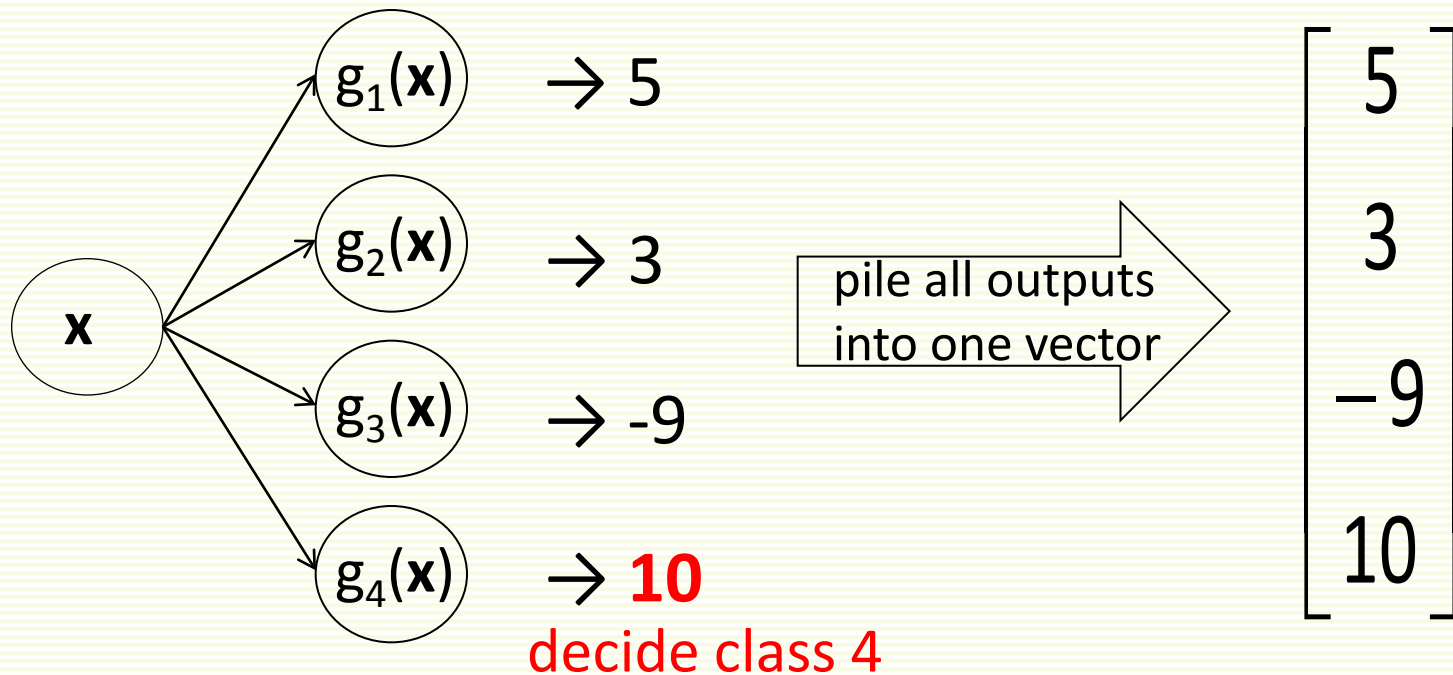


Multiclass Linear Classifier: Matrix Notation

- Assume examples \mathbf{x} are augmented with extra feature 1, no need to write bias explicitly
 - but from now on will not change notation to \mathbf{z} 's
- Define m discriminant functions

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

- Assign \mathbf{x} to i that gives maximum $\mathbf{g}_i(\mathbf{x})$
- Picture illustration



Multiclass Linear Classifier: Matrix Notation

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

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

class 1

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

class 2

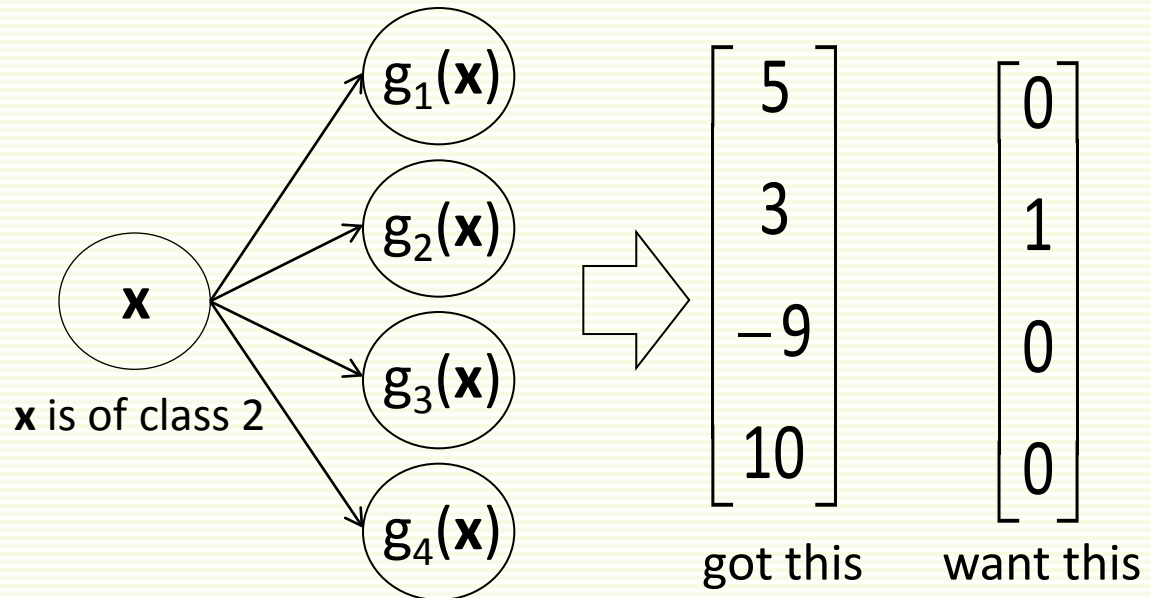
$$y^j = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

class 3

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

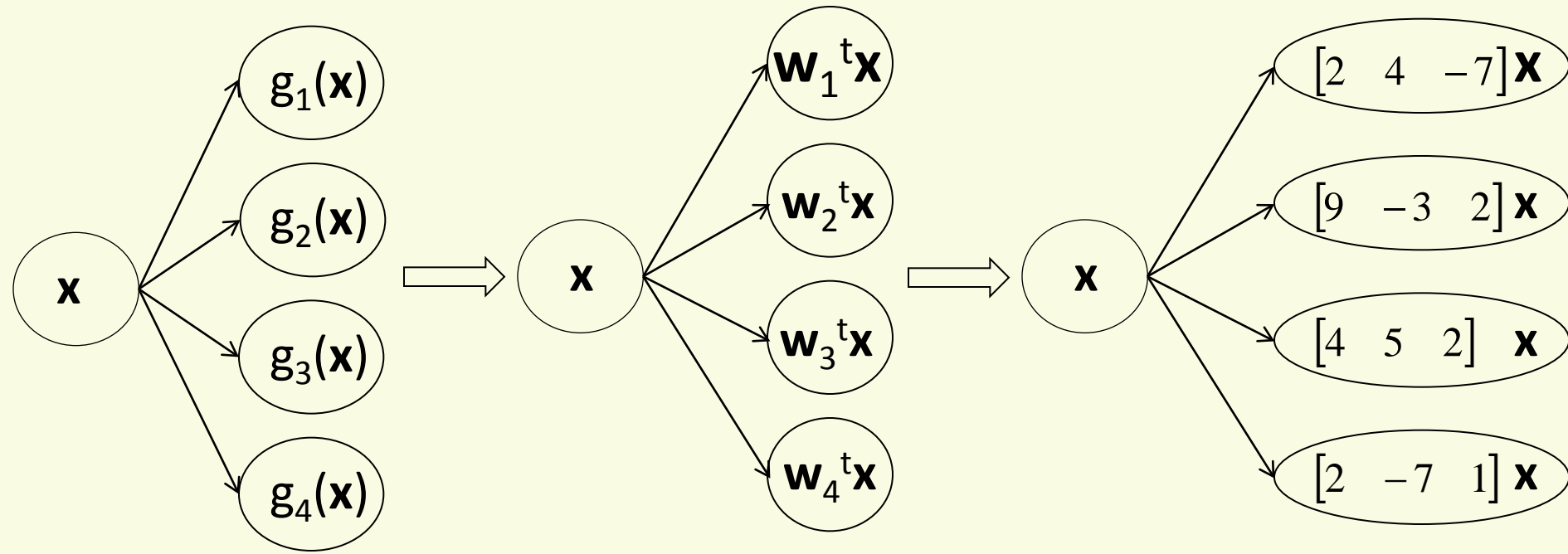
class 4

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



Multiclass Linear Classifier: Matrix Notation

- Assign \mathbf{x} to i that gives maximum $g_i(\mathbf{x}) = \mathbf{w}_i^t \mathbf{x}$



- In matrix notation

$$\begin{matrix} \mathbf{w}_1 \\ \mathbf{w}_2 \\ \mathbf{w}_3 \\ \mathbf{w}_4 \end{matrix} \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 7 \\ 4 \end{bmatrix} = \begin{bmatrix} 2 \\ -4 \\ 47 \\ -43 \end{bmatrix}$$

$\mathbf{W} \quad \mathbf{x} \quad \mathbf{Wx}$

- Assign \mathbf{x} to class that corresponds to largest row of \mathbf{Wx}

Quadratic Loss Function

- Assign sample \mathbf{x}^i to class that corresponds to largest row of $\mathbf{W}\mathbf{x}^i$
- Loss function?

$$\begin{array}{c} \left[\begin{array}{c} 2 \\ -4 \\ 47 \\ -43 \end{array} \right] \\ \mathbf{W}\mathbf{x}^i \end{array} \quad \begin{array}{c} \left[\begin{array}{c} 0 \\ 0 \\ 0 \\ 1 \end{array} \right] \\ \mathbf{y}^i \end{array}$$

- 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 $L(\mathbf{W}) = \frac{1}{2}\sum_i \|\mathbf{W}\mathbf{x}^i - \mathbf{y}^i\|^2$
 - gradient of the loss

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

- $\nabla L(\mathbf{W})$ has the same shape as the same shape as \mathbf{W}
- batch gradient descent update

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

Quadratic Loss Function

- Consider gradient descent update, single sample \mathbf{x} with $\alpha = 1$

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

- Suppose $\mathbf{x} = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix}$ and is of class 2 and $\mathbf{W} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix}$

$$\begin{array}{l} \text{ok} \\ \text{too large} \\ \text{too small} \end{array} \begin{array}{l} \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \mathbf{W}\mathbf{x} - \mathbf{y} = \begin{bmatrix} 0 \\ 4 \\ 23 \\ -17 \end{bmatrix} - \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 23 \\ -17 \end{bmatrix}$$

- update rule

$$\mathbf{W} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 3 \\ 23 \\ -17 \end{bmatrix} \begin{bmatrix} 1 & 3 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 \\ 3 & 9 & 6 \\ 23 & 69 & 46 \\ -17 & -51 & -34 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -7 \\ 6 & -12 & -4 \\ -19 & -64 & -44 \\ 19 & 44 & 35 \end{bmatrix}$$

Quadratic Loss Function

$$\begin{array}{l} \text{ok} \\ \text{too large} \\ \text{too small} \end{array} \begin{array}{l} \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \begin{bmatrix} 0 \\ 4 \\ 23 \\ -17 \end{bmatrix} - \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 23 \\ -17 \end{bmatrix}$$

$\mathbf{Wx} - \mathbf{y} =$

- With new $\mathbf{W} = \begin{bmatrix} 2 & 4 & -7 \\ 6 & -12 & -4 \\ -19 & -64 & -44 \\ 19 & 44 & 35 \end{bmatrix}$, $\mathbf{Wx} = \begin{bmatrix} 0 \\ -38 \\ -299 \\ 221 \end{bmatrix}$

- Already saw that quadratic loss does not work that well for classification

Perceptron Loss

- Generalize Perceptron loss to multiclass setting
- Per-example loss: largest score minus score for the correct class

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

$$\mathbf{Wx}^i \quad \mathbf{y}^i$$

Loss is $47 - (-43) = 90$

$$\begin{bmatrix} 20 \\ 40 \\ 17 \\ -43 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\mathbf{Wx}^i \quad \mathbf{y}^i$$

Loss is $40 - 40 = 0$

- Formula for Perceptron loss on sample \mathbf{x}^i

$$L_i(\mathbf{W}) = \max_k [(\mathbf{Wx}^i)_k - (\mathbf{Wx}^i)_c]$$

- $(\mathbf{Wx}^i)_k$ is the entry in row k of vector \mathbf{Wx}^i
- c is the correct class of sample \mathbf{x}^i

Perceptron Loss Function

- Gradient of loss on one example
 - \mathbf{c} is the correct class row
 - \mathbf{r} is the row where $\mathbf{W}\mathbf{x}^i$ is largest
 - if $\mathbf{r} = \mathbf{c}$, $-\nabla L_i(\mathbf{W}) = 0$

- otherwise, $-\nabla L_i(\mathbf{W}) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ -x^i & & & \\ 0 & 0 & 0 & 0 \\ x^i & & & \end{bmatrix}$
row \mathbf{r}
row \mathbf{c}

- Example

$$\begin{bmatrix} 2 \\ -4 \\ 47 \\ -43 \end{bmatrix} \quad \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

$\mathbf{W}\mathbf{x}^i \quad \mathbf{x}^i \quad \mathbf{y}^i$

$$-\nabla L_i(\mathbf{W}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & -3 & -2 \\ 1 & 3 & 2 \end{bmatrix}$$

Perceptron Loss Function: Example Cont.

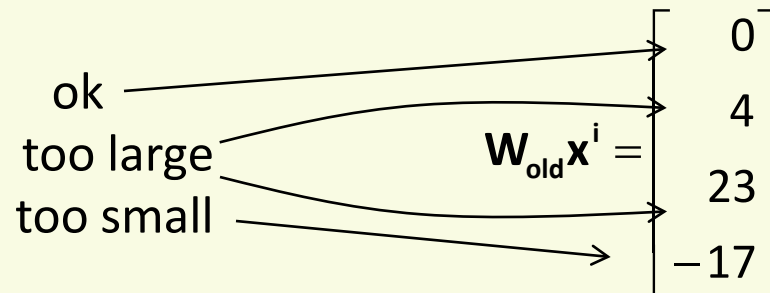
$$-\nabla L_i(\mathbf{W}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & -3 & -2 \\ 1 & 3 & 2 \end{bmatrix} \quad \mathbf{x}^i = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \quad \mathbf{y}^i = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

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

- With new weights

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

- Compare to the old weights



Softmax Function

- Define softmax(**a**) function
- Example

$$\begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \\ \mathbf{a}_4 \end{bmatrix} \xrightarrow{\text{softmax}} \begin{bmatrix} \frac{\exp(\mathbf{a}_1)}{\sum_{j=1}^4 \exp(\mathbf{a}_j)} \\ \frac{\exp(\mathbf{a}_2)}{\sum_{j=1}^4 \exp(\mathbf{a}_j)} \\ \frac{\exp(\mathbf{a}_3)}{\sum_{j=1}^4 \exp(\mathbf{a}_j)} \\ \frac{\exp(\mathbf{a}_4)}{\sum_{j=1}^4 \exp(\mathbf{a}_j)} \end{bmatrix}$$

$$\begin{bmatrix} -3 \\ 2 \\ 1 \end{bmatrix} \xrightarrow{\text{softmax}} \begin{bmatrix} \frac{\exp(-3)}{\exp(-3) + \exp(2) + \exp(1)} \\ \frac{\exp(2)}{\exp(-3) + \exp(2) + \exp(1)} \\ \frac{\exp(1)}{\exp(-3) + \exp(2) + \exp(1)} \end{bmatrix}$$

$$= \begin{bmatrix} 0.005 \\ 0.7275 \\ 0.2676 \end{bmatrix}$$

- Softmax renormalizes a vector so that it can be interpreted as a vector of probabilities

Softmax Loss Function

- Generalization of logistic regression to multiclass case

- Instead of raw scores
$$\begin{bmatrix} w_1^T \mathbf{x} \\ w_2^T \mathbf{x} \\ w_3^T \mathbf{x} \\ w_4^T \mathbf{x} \end{bmatrix} = \begin{bmatrix} 2 \\ -1 \\ 5 \\ -3 \end{bmatrix}$$

- Use softmax scores

$$\text{softmax} \left(\begin{bmatrix} w_1^T \mathbf{x} \\ w_2^T \mathbf{x} \\ w_3^T \mathbf{x} \\ w_4^T \mathbf{x} \end{bmatrix} \right) = \text{softmax} \left(\begin{bmatrix} 2 \\ -1 \\ 5 \\ -3 \end{bmatrix} \right) = \begin{bmatrix} 0.0473 \\ 0.0024 \\ 0.9500 \\ 0.0003 \end{bmatrix} = \begin{bmatrix} \text{Pr}(\text{class1}) \\ \text{Pr}(\text{class2}) \\ \text{Pr}(\text{class3}) \\ \text{Pr}(\text{class4}) \end{bmatrix}$$

- Classifier output interpreted as probability for each class

Gradient Descent: Softmax Loss Function

- Optimize under $-\log \Pr(\mathbf{y}^i)$ loss function
- Example

$$\mathbf{x}^i = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \quad \mathbf{y}^i = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \quad \mathbf{W} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix}$$

$$\text{softmax}(\mathbf{W}\mathbf{x}^i) = \text{softmax} \left(\begin{bmatrix} 0 \\ 4 \\ 23 \\ -17 \end{bmatrix} \right) = \begin{bmatrix} 0.000000000102619 \\ 0.0000000005602796 \\ 0.9999999994294585 \\ 0.0000000000000001 \end{bmatrix} = \begin{bmatrix} \text{Pr}(\text{class1}) \\ \text{Pr}(\text{class2}) \\ \text{Pr}(\text{class3}) \\ \text{Pr}(\text{class4}) \end{bmatrix}$$

- Loss on this example is $-\log(0.0000000000000001) = 40$

Gradient Descent: Softmax Loss Function

- Update rule for weight matrix \mathbf{W}

$$\mathbf{W} = \mathbf{W} + \alpha \sum_i (\mathbf{y}^i - \text{softmax}(\mathbf{W}^T \mathbf{x}^i)) (\mathbf{x}^i)^t$$

- Example, single sample gradient descent with $\alpha = 0.1$

$$\mathbf{x}^i = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \quad \mathbf{y}^i = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \quad \mathbf{W} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} \quad \mathbf{W}\mathbf{x}^i = \begin{bmatrix} 0 \\ 4 \\ 23 \\ -17 \end{bmatrix}$$

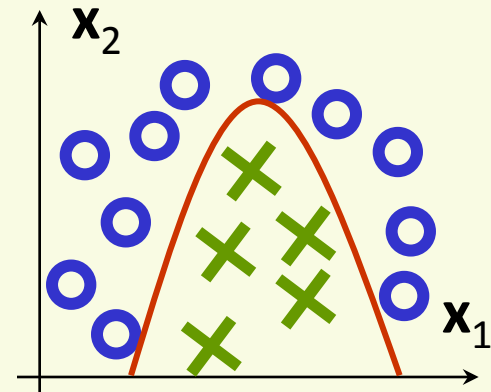
- Update for \mathbf{W}

$$\mathbf{W} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 4 & 5 & 2 \\ 2 & -7 & 1 \end{bmatrix} + 0.1 \left(\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} - \text{softmax} \begin{bmatrix} 0 \\ 4 \\ 23 \\ -17 \end{bmatrix} \right) \begin{bmatrix} 1 & 3 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -7 \\ 9 & -3 & 2 \\ 3.9 & 4.7 & 1.8 \\ 2.1 & -6.7 & 1.2 \end{bmatrix}$$

Generalized Linear Classifier

- Can use other discriminant functions, like quadratics

$$g(\mathbf{x}) = \mathbf{w}_0 + \mathbf{w}_1 \mathbf{x}_1 + \mathbf{w}_2 \mathbf{x}_2 + \mathbf{w}_{12} \mathbf{x}_1 \mathbf{x}_2 + \mathbf{w}_{11} \mathbf{x}_1^2 + \mathbf{w}_{22} \mathbf{x}_2^2$$



- Methodology is almost the same as in the linear case

- $\mathbf{f}(\mathbf{x}) = \text{sign}(\mathbf{w}_0 + \mathbf{w}_1 \mathbf{x}_1 + \mathbf{w}_2 \mathbf{x}_2 + \mathbf{w}_{12} \mathbf{x}_1 \mathbf{x}_2 + \mathbf{w}_{11} \mathbf{x}_1^2 + \mathbf{w}_{22} \mathbf{x}_2^2)$
- $\mathbf{z} = [1 \quad \mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_1 \mathbf{x}_2 \quad \mathbf{x}_1^2 \quad \mathbf{x}_2^2]$
- $\mathbf{a} = [\mathbf{w}_0 \quad \mathbf{w}_1 \quad \mathbf{w}_2 \quad \mathbf{w}_{12} \quad \mathbf{w}_{11} \quad \mathbf{w}_{22}]$
- use gradient descent to minimize Perceptron loss function, any other loss function
- Can add any degree polynomial features

Generalized Linear Classifier

- Generalized linear classifier

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

- $\mathbf{h}(\mathbf{x})$ are called basis function, can be arbitrary functions
 - in strictly linear case, $\mathbf{h}_i(\mathbf{x}) = \mathbf{x}_i$

- Linear function in its parameters \mathbf{w}

$$\mathbf{g}(\mathbf{x}, \mathbf{w}) = \mathbf{w}_0 + \mathbf{w}^t \mathbf{h}$$

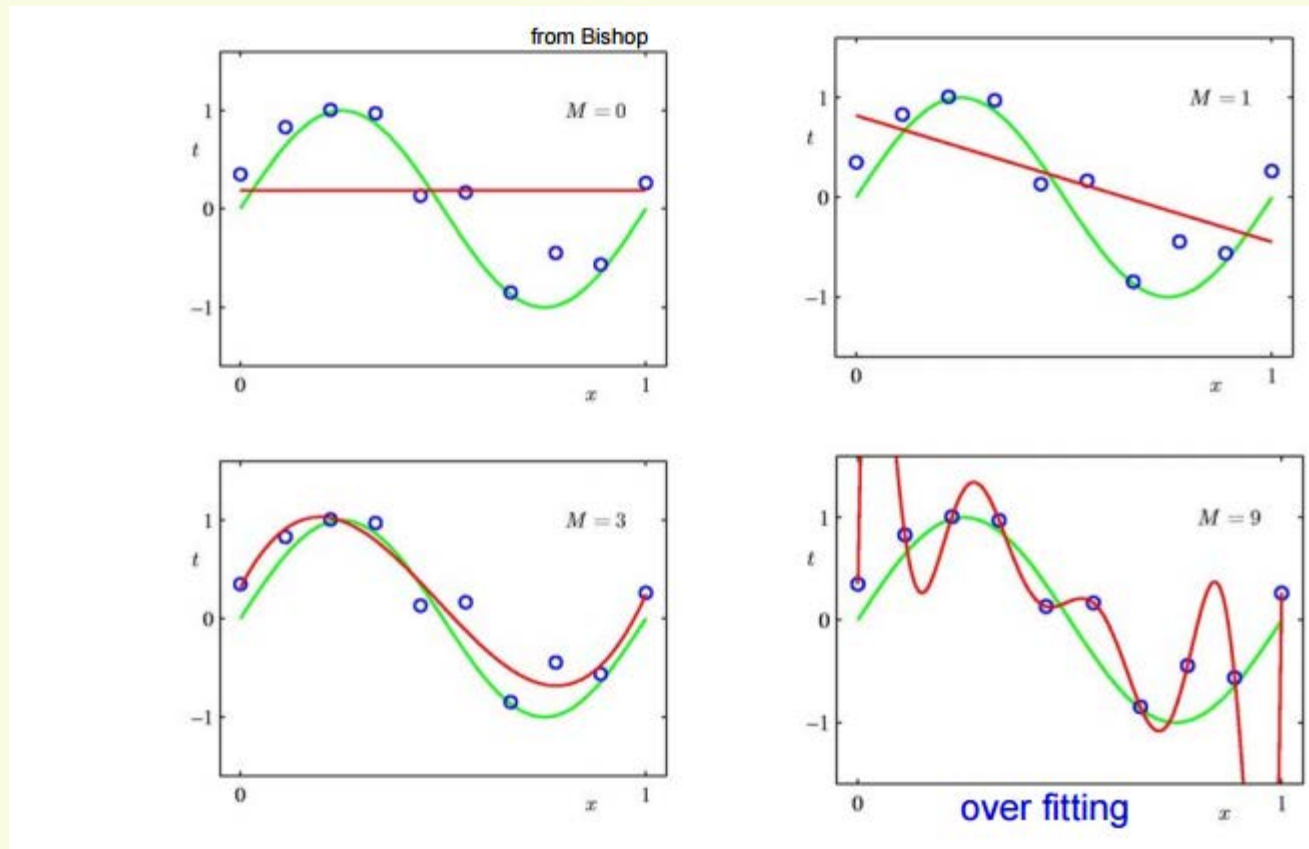
$$\mathbf{h} = [\mathbf{h}_1(\mathbf{x}) \quad \mathbf{h}_2(\mathbf{x}) \quad \dots \quad \mathbf{h}_m(\mathbf{x})]$$

$$[\mathbf{w}_1 \quad \mathbf{w}_2 \quad \dots \quad \mathbf{w}_m]$$

- Use the same training methods as before with new feature vector \mathbf{h}

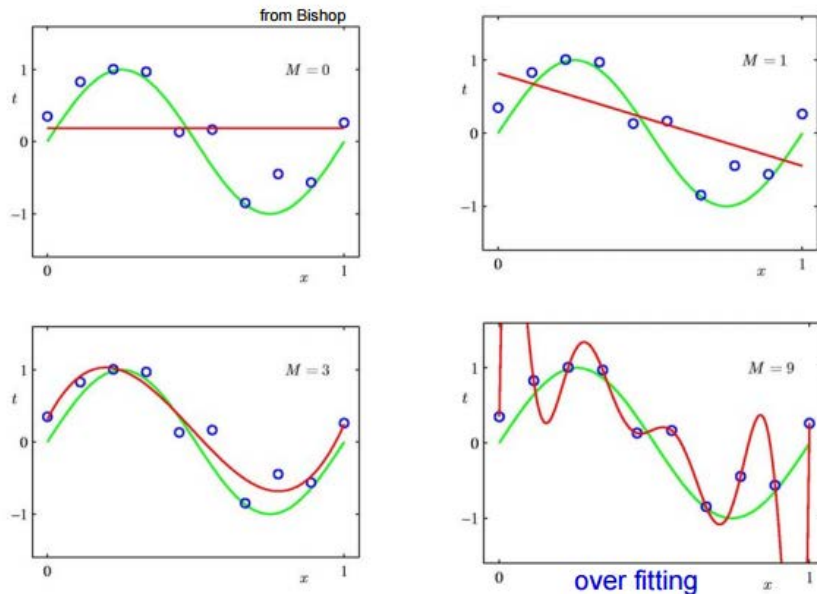
Generalized Linear Classifier

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



Generalized Linear Classifier

- Helps to regularize by keeping \mathbf{w} small
 - small \mathbf{w} means the boundary is not as curvy
- Regression example



Polynomial Coefficients

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
w_0^*	0.19	0.82	0.31	0.35
w_1^*		-1.27	7.99	232.37
w_2^*			-25.43	-5321.83
w_3^*			17.37	48568.31
w_4^*				-231639.30
w_5^*				640042.26
w_6^*				-1061800.52
w_7^*				1042400.18
w_8^*				-557682.99
w_9^*				125201.43

Generalized Linear Classifier

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

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

- Regularized version

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

- Regression example, polynomial coefficients for degree $M = 9$
- With weight regularizer, gradient of loss function has a new term $-\alpha \lambda \mathbf{w}$

	small λ	medium λ	large λ
w_0^*	0.35	0.35	0.13
w_1^*	232.37	4.74	-0.05
w_2^*	-5321.83	-0.77	-0.06
w_3^*	48568.31	-31.97	-0.05
w_4^*	-231639.30	-3.89	-0.03
w_5^*	640042.26	55.28	-0.02
w_6^*	-1061800.52	41.32	-0.01
w_7^*	1042400.18	-45.95	-0.00
w_8^*	-557682.99	-91.53	0.00
w_9^*	125201.43	72.68	0.01

Generalized Linear Classifier

- λ is a meta-parameter, cannot tune on training data
 - use validation or cross-validation to set it to a good value
- Consider polynomial of degree $M=9$ regression

