#### Logistic Regression

Machine Learning – CSEP546
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University of Washington

January 27, 2014

#### Reading Your Brain, Simple Example

[Mitchell et al.] Pairwise classification accuracy: 85% Person Animal

#### Classification

>X = (GPA, grade, resum, )

- Learn: h:X → Y
  - □ X features
  - ☐ Y target classes

Simplest case: Thresholding

X: Load Comparks

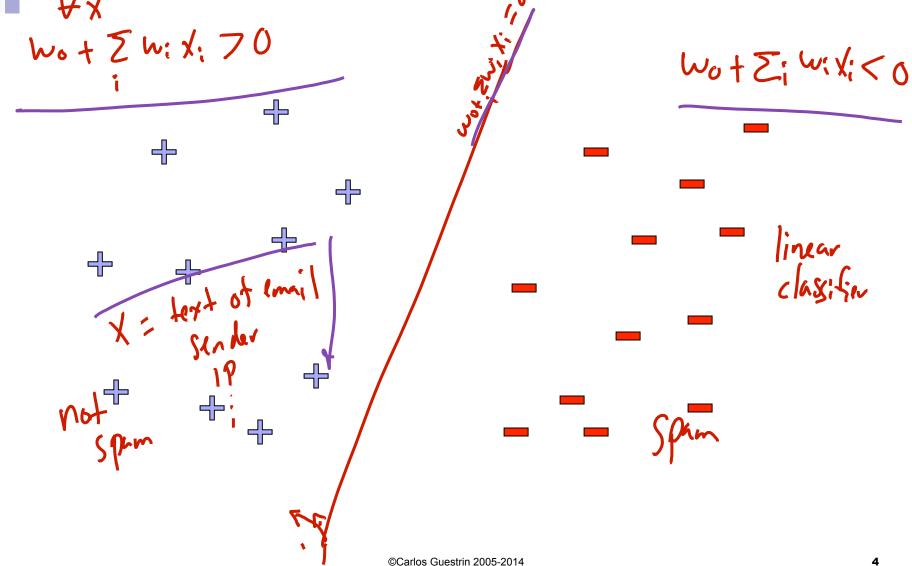
Y=alarm?

Load 799% => alarm = form Xi 1/5e -> alarm = fals

Xj>. 27°C

Linear (Hyperplane) Decision

Roundaries work 2 works o **Boundaries** 



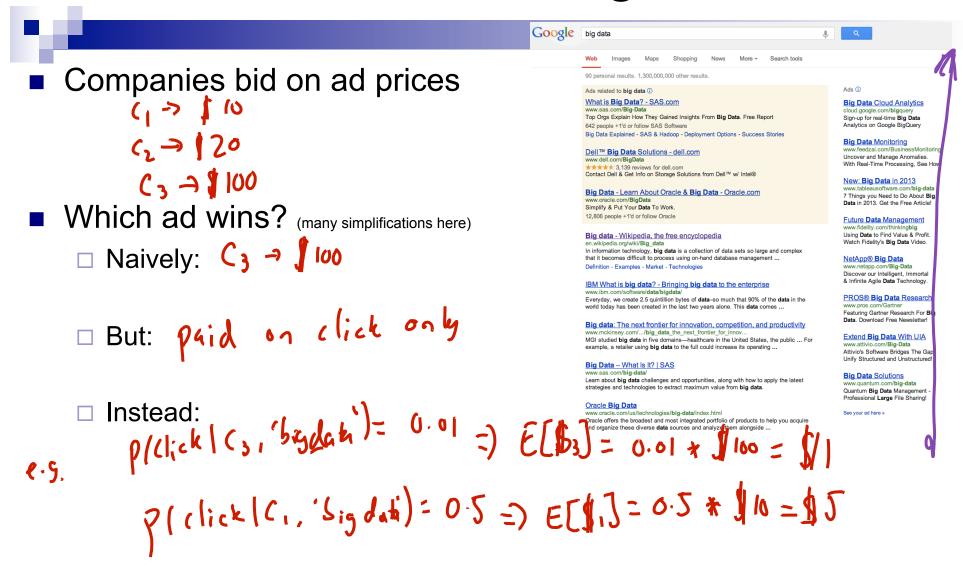
#### Classification



- Learn: h:X → Y
  - □ X features
  - ☐ Y target classes
- Thus far: just a decision boundary

What if you want probability of each class? P(Y|X)

#### Ad Placement Strategies



#### Link Functions



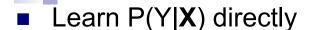
[0,1] P(Y|X) - 20012 R

- Combing regression and probability?
  - □ Need a mapping from real values to [0,1]
  - □ A link function!

#### Logistic Regression

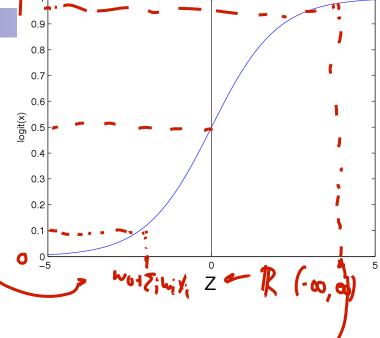
Logistic **function** (or Sigmoid):

$$\frac{1}{1 + exp(-z)}$$



- Assume a particular functional form for link function
- Sigmoid applied to a linear function of the input features:

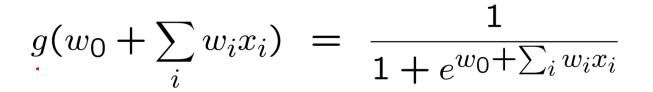
features: 
$$P(Y=0|X,W) = \frac{1}{1 + exp(w_0 + \sum_i w_i X_i)}$$



Features can be discrete or continuous! ©Carlos Guestrin 2005-2014

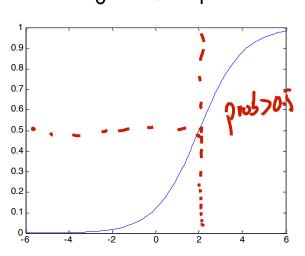
#### Understanding the sigmoid

w, ... wa = 0

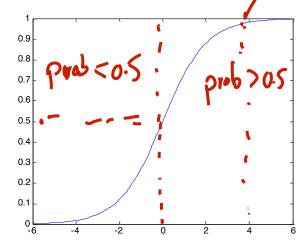


Shift

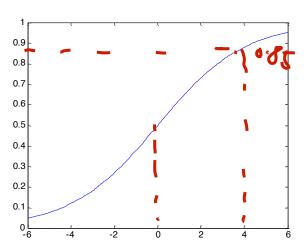
$$W_0 = -2, W_1 = -1$$







$$w_0 = 0, w_1 = -0.5$$



#### Logistic Regression a Linear classifier

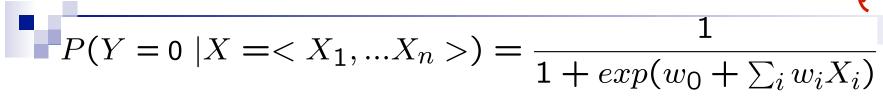
$$\frac{1}{1 + exp(-z)} \begin{bmatrix} 0.9 \\ 0.8 \\ 0.7 \\ 0.6 \\ 0.5 \\ 0.4 \\ 0.3 \\ 0.2 \end{bmatrix}$$

#### P(4=0/W,x)=

$$g(w_0 + \sum_i w_i x_i) = \frac{1}{1 + e^{w_0 + \sum_i w_i x_i}}$$

$$\rho(y=0|w,x)<0.5$$

#### Very convenient!



implies

$$P(Y = 1 \mid X = < X_1, ...X_n >) = \frac{exp(w_0 + \sum_i w_i X_i)}{1 + exp(w_0 + \sum_i w_i X_i)}$$

implies

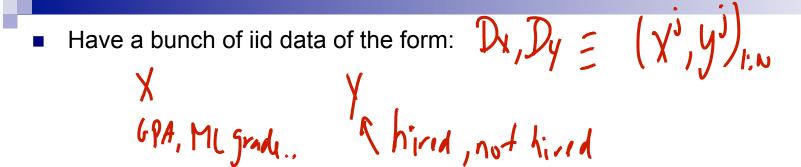
$$\frac{P(Y = 1 | X)}{P(Y = 0 | X)} = exp(w_0 + \sum_{i} w_i X_i)$$

implies 
$$P(Y = 1 \mid X) = w_0 + \sum_i w_i X_i > 0$$

linear classification rule!

#### X) = ith dimension of jth detapoint

#### Loss function: Conditional Likelihood



Discriminative (logistic regression) loss function:

Conditional Data Likelihood

$$P(D_y | D_x, w) = 9rsmx$$
 $P(y | x^j, w)$ 
 $P(y | x^j, w)$ 

hrymax 
$$\ln P(\mathcal{D}_Y \mid \mathcal{D}_\mathbf{X}, \mathbf{w}) = \sum_{j=1}^N \ln P(y^j \mid \mathbf{x}^j, \mathbf{w}) - params$$

$$j \mid \mathbf{x}^j, \mathbf{w} \mid \mathbf{x}^j$$

#### **Expressing Conditional Log Likelihood**

$$l(\mathbf{w}) \equiv \sum_{j=1}^{N} \ln P(y^j | \mathbf{x}^j, \mathbf{w})$$

$$P(Y = 0 | \mathbf{X}, \mathbf{w}) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$P(Y = 1 | \mathbf{X}, \mathbf{w}) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

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$$P(Y = 1 | \mathbf{X}, \mathbf{w}) = \frac{\exp(w_0 + \sum_i w$$

#### Maximizing Conditional Log Likelihood

$$P(Y = 0|X, W) = \frac{1}{1 + exp(w_0 + \sum_i w_i X_i)}$$

$$P(Y = 1|X, W) = \frac{exp(w_0 + \sum_i w_i X_i)}{1 + exp(w_0 + \sum_i w_i X_i)}$$

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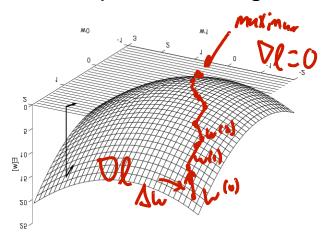
Good news:  $I(\mathbf{w})$  is concave function of  $\mathbf{w}$ , no local optima V problems

Bad news: no closed-form solution to maximize *I*(w)

Good news: concave functions easy to optimize

#### Optimizing concave function – Gradient ascent

Conditional likelihood for Logistic Regression is concave. Find optimum with gradient ascent



Gradient: 
$$abla_{\mathbf{w}} l(\mathbf{w}) = [\frac{\partial l(\mathbf{w})}{\partial w_0}, \dots, \frac{\partial l(\mathbf{w})}{\partial w_n}]'$$

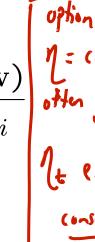
**Update rule:** 

$$\Delta \mathbf{w} = \eta \nabla_{\mathbf{w}} l(\mathbf{w})$$

rule: 
$$\Delta \mathbf{w} = \eta \nabla_{\mathbf{w}} l(\mathbf{w})$$

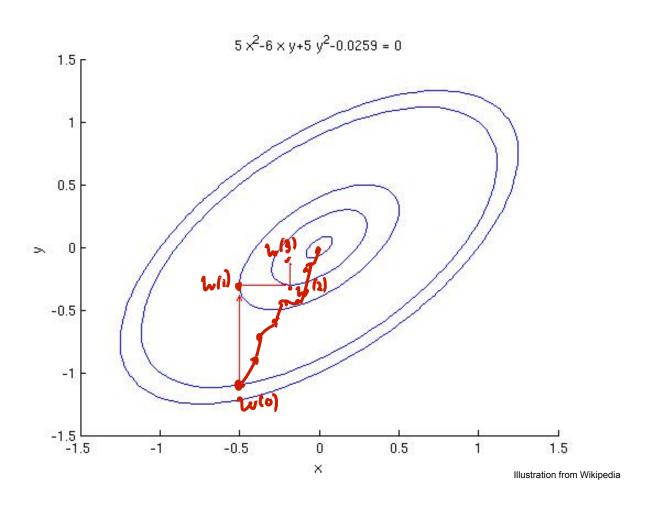
$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \frac{\partial l(\mathbf{w})}{\partial w_i}$$

- Gradient ascent is simplest of optimization approaches
  - e.g., Conjugate gradient ascent can be much better



#### Coordinate Descent v. Gradient Descent





### Maximize Conditional Log Likelihood: Gradient ascent

$$P(Y = 1|X, W) = \frac{exp(w_0 + \sum_i w_i X_i)}{1 + exp(w_0 + \sum_i w_i X_i)}$$

$$l(\mathbf{w}) = \sum_{j} y^{j}(w_{0} + \sum_{i}^{n} w_{i}x_{i}^{j}) - \ln(1 + exp(w_{0} + \sum_{i}^{n} w_{i}x_{i}^{j}))$$

$$\frac{\partial \ell(\mathbf{w})}{\partial w_{i}} = \sum_{j=1}^{N} x_{i}^{j}(y^{j} - P(Y = 1 | x^{j}, \mathbf{w}))$$

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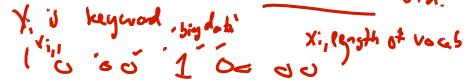
$$\frac{\partial \ell(\mathbf{w})}{\partial w_{i}} = \sum_{j=1}^{N} x_{i}^{j}(y^{j} - P(Y = 1 | x^{j}, \mathbf{w}))$$

Gradient Descent for LR: Intuition



Gender (F=1, M=0)	Age (Young=0, Middle=1, Old=2)	Location (US=1, Abroad=0)	Income (High=1, Low=0)	Refer	rer	is.	New or Returning (New=1,, Returning =0)	Clicked? (Click=1, NoClick=0)
1	O	1	1	1	0	0		0
0	1	1	O	U	0	Í	1	O
1	2	0	0	1	0	0	ð	١
6	0	0	O	J	1	0	0	0

Encode data as numbers



- Until convergence: for each feature
  - Compute average gradient over data points

b. Update parameter 
$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_{j \in I} x_i^j [y^j - \hat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w})]$$

#### Gradient Ascent for LR





$$w_0^{(t+1)} \leftarrow w_0^{(t)} + \eta \sum_{j \in I}^{N} [y^j - \hat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})]$$

For i=1,...,k, 
$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_{j \geq 1} x_i^j [y^j - \hat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})]$$

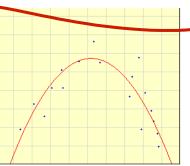
repeat

#### Regularization in linear regression

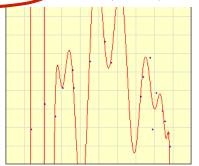


Overfitting usually leads to very large parameter choices, e.g.:

$$-2.2 + 3.1 X - 0.30 X^2$$



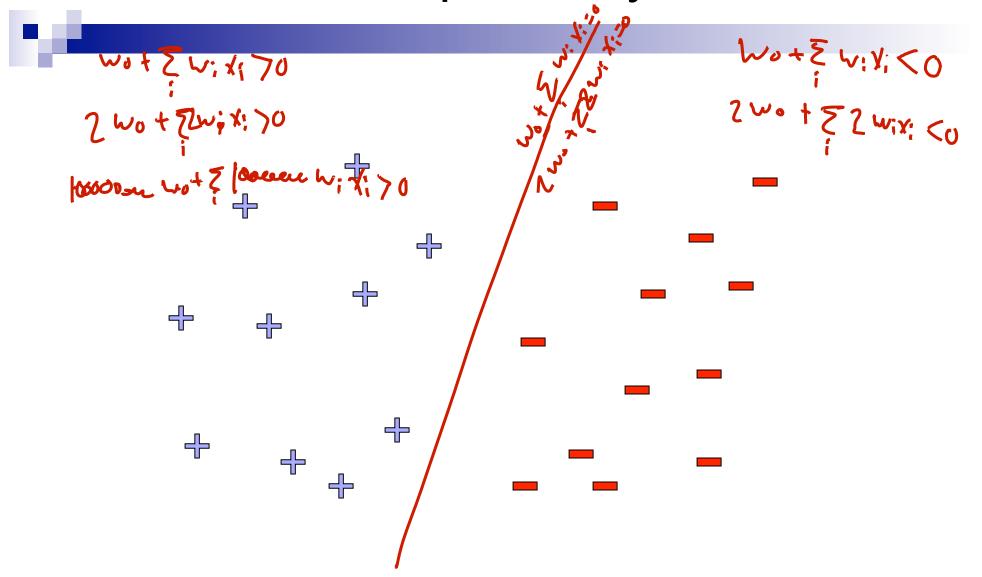
$$-1.1 + 4,700,910.7 \times -8,585,638.4 \times^2 + \dots$$



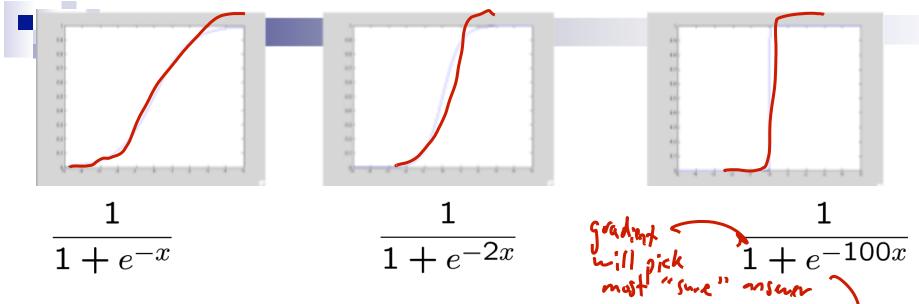
■ Regularized least-squares (a.k.a. ridge regression), for  $\lambda$ >0:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_{j} \left( t(\mathbf{x}_j) - \sum_{i} w_i h_i(\mathbf{x}_j) \right)^2 + \lambda \sum_{i=1}^k w_i^2$$

#### **Linear Separability**



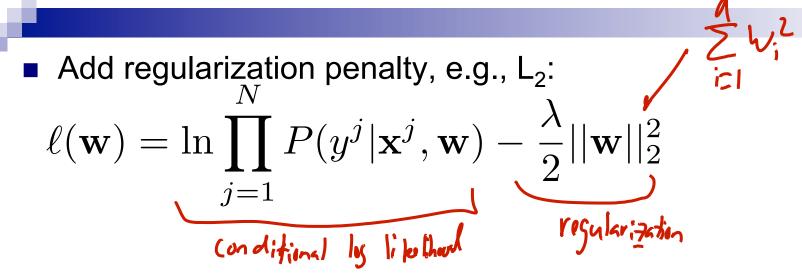
#### Large parameters → Overfitting



If data is linearly separable, weights go to infinity

- ☐ In general, leads to overfitting:
- Penalizing high weights can prevent overfitting...

#### Regularized Conditional Log Likelihood



■ Practical note about w<sub>0</sub>:

#### Standard v. Regularized Updates

Maximum conditional likelihood estimate

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \quad \ln\prod_{j=1} P(y^j | \mathbf{x}^j, \mathbf{w})$$

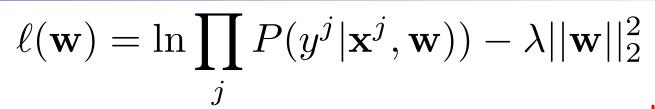
$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_j x_i^j [y^j - \hat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})]$$

Regularized maximum conditional likelihood estimate

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \prod_{j=1}^{N} P(y^j | \mathbf{x}^j, \mathbf{w}) - \frac{\lambda}{2} \sum_{i=1}^{k} w_i^2$$

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \left\{ -\lambda w_i^{(t)} + \sum_j x_i^j [y^j - \widehat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})] \right\}$$

#### Please Stop!! Stopping criterion



■ When do we stop doing gradient descent? when do we stop doing gradient descent?

$$\ell(w^*) - \ell(w^{(*)}) \leq \varepsilon$$

- Because *l*(**w**) is strongly concave:
  - □ i.e., because of some technical condition

$$\ell(\mathbf{w}^*) - \ell(\mathbf{w}^{(t)}) \leq \frac{1}{2\lambda} ||\nabla \ell(\mathbf{w})||_2^2 \quad \leq \mathcal{E} \quad \text{where } \lambda$$

■ Thus, stop when:

$$\|\nabla \varrho(\omega^{(4)})\|_{2}^{2} \leq 2\lambda \varepsilon$$

 $\|\nabla \mathcal{L}(w)\|_{2}^{2} = \frac{2}{\pi} \left(\frac{\partial \mathcal{L}}{\partial w_{i}}\right)^{2}$ 

### Digression: Logistic regression for more than 2 classes

Logistic regression in more general case (C classes), where Y in {0,...,C-1}

### Digression: Logistic regression more generally

Logistic regression in more general case, where Y in {0,...,C-1}

for 
$$c>0$$

$$P(Y = c|\mathbf{x}, \mathbf{w}) = \frac{\exp(w_{c0} + \sum_{i=1}^{k} w_{ci}x_i)}{1 + \sum_{c'=1}^{C-1} \exp(w_{c'0} + \sum_{i=1}^{k} w_{c'i}x_i)}$$

for c=0 (normalization, so no weights for this class)

$$P(Y = 0 | \mathbf{x}, \mathbf{w}) = \frac{1}{1 + \sum_{c'=1}^{C-1} \exp(w_{c'0} + \sum_{i=1}^{k} w_{c'i} x_i)}$$

Learning procedure is basically the same as what we derived!

# Stochastic Gradient Descent

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University of Washington

January 27, 2014 ©Carlos Guestrin 2005-2014

# The Cost, The Cost!!! Think about the cost...

What's the cost of a gradient update step for LR???

$$w_{i}^{(t+1)} \leftarrow w_{i}^{(t)} + \eta \left\{ -\lambda w_{i}^{(t)} + \sum_{j=1}^{N} x_{i}^{j} [y^{j} - \hat{P}(Y^{2} = 1 \mid \mathbf{x}^{j}, \mathbf{w}^{(t)})] \right\}$$

$$(ache p(Y=1 \mid \mathbf{N}, \mathbf{w}^{(t)}) \qquad O(\mathbf{N}\mathbf{k}) \quad \text{proposed for the following positions of the first of the following proposed in the proposed per positions of the proposed per positions of the first of the per position of the proposed per positions of the per position of the$$

#### Learning Problems as Expectations



- Minimizing loss in training data:
  - □ Given dataset: X', X', ....,
    - Sampled iid from some distribution p(x) on features:
  - Loss function, e.g., squared error, logistic loss,...

We often minimize loss in training data: 
$$\ell_{\mathcal{D}}(\mathbf{w}) = \frac{1}{N} \sum_{j=1}^{N} \ell(\mathbf{w}, \mathbf{x}^j) \qquad \ell(\mathbf{w}, \mathbf{x}^j) = \left( \frac{1}{N} (\mathbf{x}^j) - \left( \frac{1}{N} (\mathbf{x}$$

However, we should really minimize expected loss on all data:

$$\ell(\mathbf{w}) = E_{\mathbf{x}} \left[ \ell(\mathbf{w}, \mathbf{x}) \right] = \int p(\mathbf{x}) \ell(\mathbf{w}, \mathbf{x}) d\mathbf{x}$$

So, we are approximating the integral by the average on the training data

#### SGD: Stochastic Gradient Ascent (or Descent)



"True" gradient:

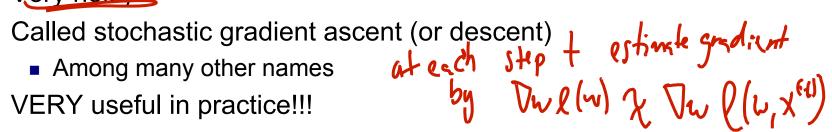
$$\nabla \ell(\mathbf{w}) = E_{\mathbf{x}} \left[ \nabla \ell(\mathbf{w}, \mathbf{x}) \right]$$

Sample based approximation:

$$\nabla_{w} \ell(w) \gtrsim \sum_{i=1}^{n} \nabla_{w} \ell(w, x^{i})$$

- What if we estimate gradient with just one sample???
  - Unbiased estimate of gradient
  - □ Very noisy!

  - VERY useful in practice!!!



### Stochastic Gradient Ascent for 6 5-100 dataping to Regression Logistic Regression

Logistic loss as a stochastic function:

$$E_{\mathbf{x}}\left[\ell(\mathbf{w},\mathbf{x})\right] = E_{\mathbf{x}}\left[\ln P(y|\mathbf{x},\mathbf{w}) - \lambda||\mathbf{w}||_2^2\right]$$
Batch gradient ascent updates:
$$(t+1) \quad (t) \quad \left\{ \begin{array}{ccc} (t) & 1 & \sum_{i=1}^{N} f(i) \cdot f(i) & f(i) \end{array} \right.$$

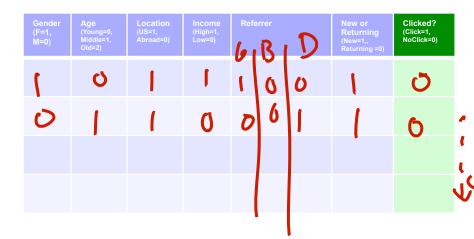
$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \left\{ -\lambda w_i^{(t)} + \frac{1}{N} \sum_{j=1}^N x_i^{(j)} [y^{(j)} - P(Y = 1 | \mathbf{x}^{(j)}, \mathbf{w}^{(t)})] \right\}$$

- Stochastic gradient ascent updates: wył example (x(4),y(4))
  - □ Online setting: ←

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta_t \left\{ -\lambda w_i^{(t)} + x_i^{(t)} [y^{(t)} - P(Y = 1 | \mathbf{x}^{(t)}, \mathbf{w}^{(t)})] \right\}$$

## Stochastic Gradient Descent for LR: Intuition





- Until convergence: get a data point
  - a. Encode data as numbers
  - b. For each feature
    - i. Compute gradient for this data point
    - ii. Update parameter

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta_t \left\{ -\lambda w_i^{(t)} + x_i^{(t)} [y^{(t)} - P(Y = 1 | \mathbf{x}^{(t)}, \mathbf{w}^{(t)})] \right\}$$

#### Stochastic Gradient Ascent: general case

- Given a stochastic function of parameters:
  - Want to find maximum

- Start from  $\mathbf{w}^{(0)} \leftarrow \mathbf{c}^{(0)}$
- Repeat until convergence:
  - Get a sample data point **x**<sup>t</sup>
  - Update parameters:

pdate parameters:
$$w_{i}^{(t+1)} \vdash w_{i}^{(t)} + \chi_{t} \frac{\partial}{\partial w_{i}} \mathcal{L}(w_{i}^{(t)}, \chi_{t}^{t})$$

- Works on the online learning setting!
- Complexity of each gradient step is constant in number of examples!
- In general, step size changes with iterations

(w) ~ [ = [w,xi)

#### What you should know...



- Classification: predict discrete classes rather than real values
- Logistic regression model: Linear model
  - □ Logistic function maps real values to [0,1]
- Optimize conditional likelihood
- Gradient computation
- Overfitting
- Regularization
- Regularized optimization
- Cost of gradient step is high, use stochastic gradient descent

# What's the Perceptron Optimizing?

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## Remember our friend the Perceptron Algorithm

- At each time step:
  - ☐ Observe a data point:

$$X^{t},y^{t}$$
  $S^{t} = Sign(w.x^{t})$ 

□ Update parameters if make a mistake:

if 
$$\hat{y}^{\dagger} \ddagger \hat{y}^{\dagger}$$

$$w(t) = w(t)$$

$$e|g(t)|_{W(t+1)} = w(t)$$

### What is the Perceptron Doing???

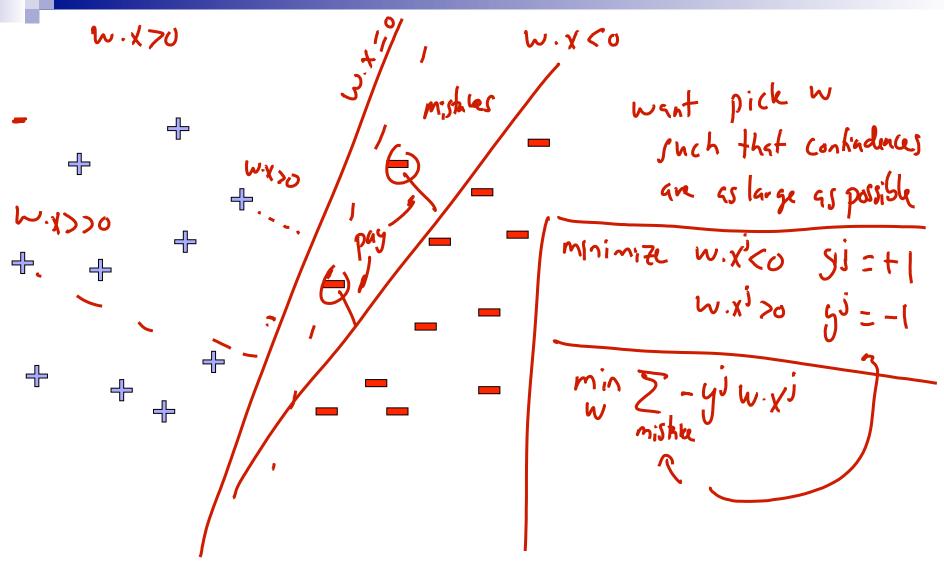


- When we discussed logistic regression:
  - Started from maximizing conditional log-likelihood

- When we discussed the Perceptron:
  - Started from description of an algorithm

What is the Perceptron optimizing????

## Perceptron Prediction: Margin of Confidence



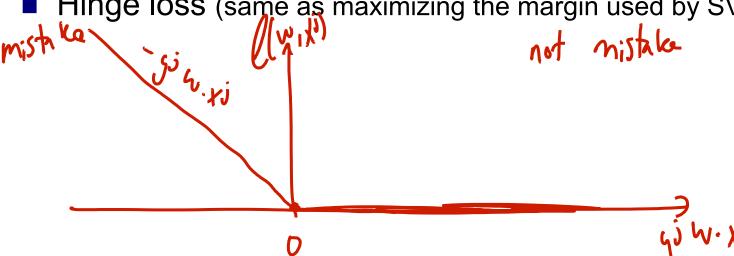
### Hinge Loss



Makes a mistake when:

$$\mathcal{L}(w,x^{i}) = \begin{cases} 0 & \text{if } w.x^{i} > 0 \\ -y^{i}w.x^{i} & \text{if } x \end{cases}$$

Hinge loss (same as maximizing the margin used by SVMs)



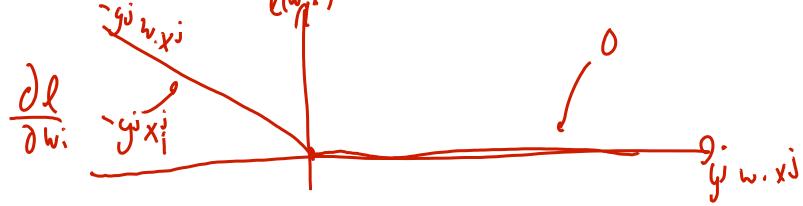
#### Stochastic Gradient Descent for Hinge Loss



■ SGD: observe data point x<sup>(t)</sup>, update each parameter

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \eta_t \frac{\partial \ell(\mathbf{w}^{(t)}, x^{(t)})}{\partial w_i}$$

How do we compute the gradient for hinge loss?



### (Sub)gradient of Hinge



$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \eta_t \frac{\partial \ell(\mathbf{w}^{(t)}, x^{(t)})}{\partial w_i}$$

Subgradient of hinge loss:

#### Stochastic Gradient Descent for Hinge Loss



SGD: observe data point x<sup>(t)</sup>, update each parameter

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \eta_t \frac{\partial \ell(\mathbf{w}^{(t)}, x^{(t)})}{\partial w_i}$$

How do we compute the gradient for hinge loss?

### Perceptron Revisited

SGD for hinge loss



$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + \mathbf{w}^{(t)} \left[ y^{(t)} (\mathbf{w}^{(t)} \cdot \mathbf{x}^{(t)}) \le 0 \right] y^{(t)} \mathbf{x}^{(t)}$$

Perceptron update:

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + \mathbb{1} \left[ y^{(t)} (\mathbf{w}^{(t)} \cdot \mathbf{x}^{(t)}) \le 0 \right] y^{(t)} \mathbf{x}^{(t)}$$

Difference?

#### What you need to know

- - Perceptron is optimizing hinge loss
  - Subgradients and hinge loss
  - (Sub)gradient decent for hinge objective

# Support Vector Machines

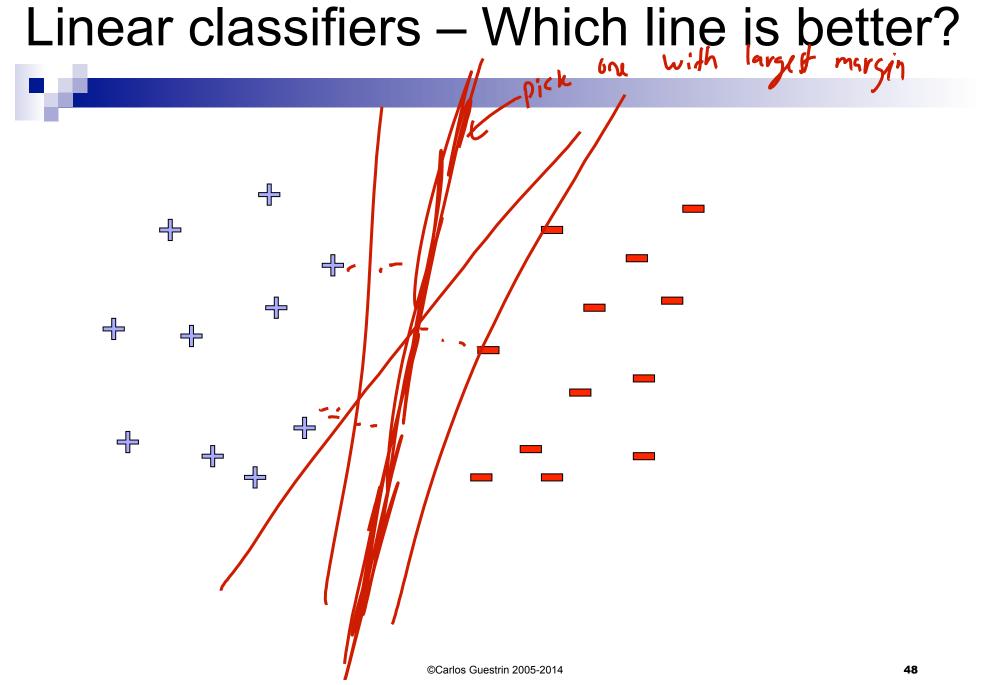
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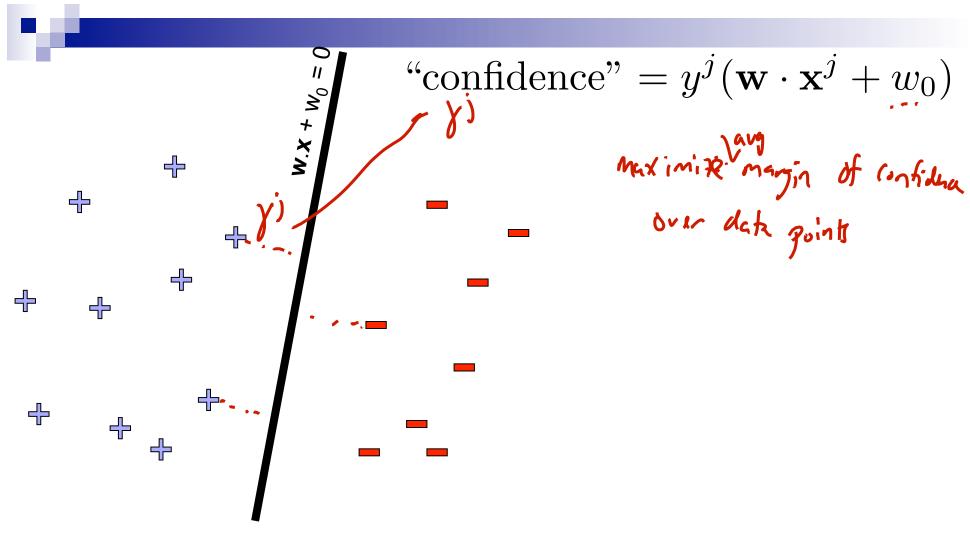
#### Support Vector Machines



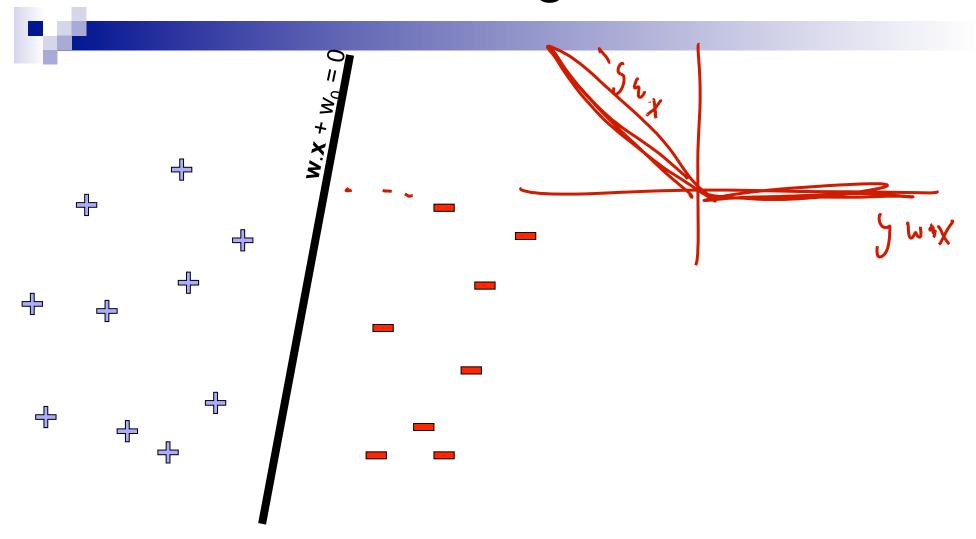
- One of the most effective classifiers to date!
- Popularized kernels
- There is a complicated derivation, but...
- Very simple based on what you've learned thus far!



### Pick the one with the largest margin!



## Maximize the margin

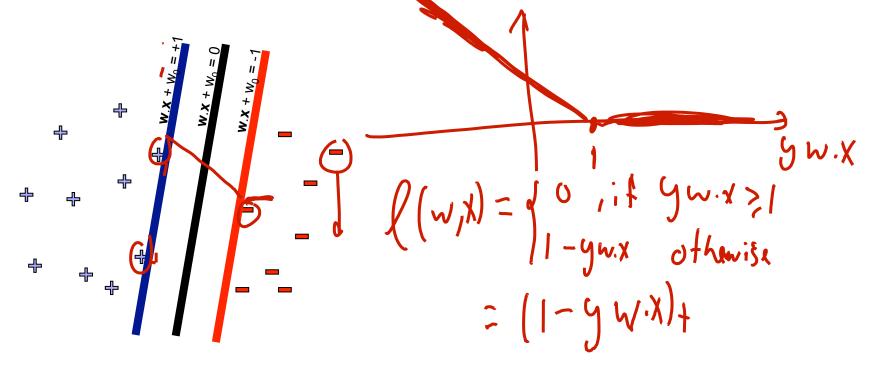


#### SVMs = Hinge Loss + L2 Regularization

(a) + : { a if q>0

Maximizing Margin same as regularized hinge loss

But, SVM "convention" is confidence has to be at least 1...



## L2 Regularized Hinge Loss



Final objective, adding regularization:

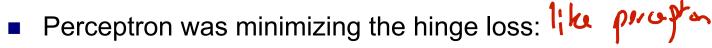


$$+$$
  $\frac{\lambda}{2} \| w \|_{2}^{2}$ 

But, again, in SVMs, convention slightly different (but equivalent)

$$\frac{||\mathbf{w}||_{2}^{2}}{2} + C \sum_{j=1}^{N} (1 - y^{j} (\mathbf{w} \cdot \mathbf{x}^{j} + w_{0}))_{+}$$

## SVMs for Non-Linearly Separable meet my friend the Perceptron...



$$\sum_{j=1}^{N} \left( -y^{j} (\mathbf{w} \cdot \mathbf{x}^{j} + w_{0}) \right)_{+}$$

SVMs minimizes the regularized hinge loss!!

$$||\mathbf{w}||_2^2 + C \sum_{j=1}^N \left(1 - y^j (\mathbf{w} \cdot \mathbf{x}^j + w_0)\right)_+$$

#### Stochastic Gradient Descent for SVMs



#### Perceptron minimization:

$$\sum_{j=1}^{N} \left( -y^{j} (\mathbf{w} \cdot \mathbf{x}^{j} + w_{0}) \right)_{+}$$

SGD for Perceptron:

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + \mathbb{1}\left[y^{(t)}(\mathbf{w}^{(t)} \cdot \mathbf{x}^{(t)}) \leq 0\right] y^{(t)}\mathbf{x}^{(t)}$$

**SVMs** minimization:

$$||\mathbf{w}||_{2}^{2} + C \sum_{j=1}^{N} (1 - y^{j} (\mathbf{w} \cdot \mathbf{x}^{j} + w_{0}))_{+}$$

#### What you need to know

- .
  - Maximizing margin
  - Derivation of SVM formulation
  - Non-linearly separable case
    - ☐ Hinge loss
    - □ A.K.A. adding slack variables
  - SVMs = Perceptron + L2 regularization
  - Can also use kernels with SVMs
  - Can optimize SVMs with SGD
    - Many other approaches possible

## Boosting

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#### Fighting the bias-variance tradeoff

- r,e
  - Simple (a.k.a. weak) learners are good
    - □ e.g., naïve Bayes, logistic regression, decision stumps (or shallow decision trees)
    - □ Low variance, don't usually overfit too badly
  - Simple (a.k.a. weak) learners are bad
    - ☐ High bias, can't solve hard learning problems



- Can we make weak learners always good???
  - □ No!!!
  - But often yes…

## The Simplest Weak Learner: Thresholding, a.k.a. Decision Stumps

X = (6PA, grade,... Learn: h:X → Y □ X – features □ Y - target classes - Ythick, not hind) Simplest case: Thresholding 1/6 h(x) = { hird if 6PA7 3.9 Not kind, others

### Voting (Ensemble Methods)

- Instead of learning a single (weak) classifier, learn many weak classifiers that are h:: x -> 1 € 1-1,+17 good at different parts of the input space
- Output class: (Weighted) vote of each classifier
  - Classifiers that are most "sure" will vote with more conviction
  - Classifiers will be most "sure" about a particular part of the space
  - On average, do better than single classifier!

H(X) = 
$$\lim_{t\to\infty} \left( \frac{1}{t} + \frac{1}{t} \right)$$
 [that sont e.g.  $h_t(x) = GPA > 3.9$ ?

- force classifiers to learn about different parts of the input space?
- weigh the votes of different classifiers?