### **Case Study 1: Estimating Click Probabilities**

# Intro Logistic Regression Gradient Descent + SGD

Machine Learning for Big Data CSE547/STAT548, University of Washington Sham Kakade March 28, 2017

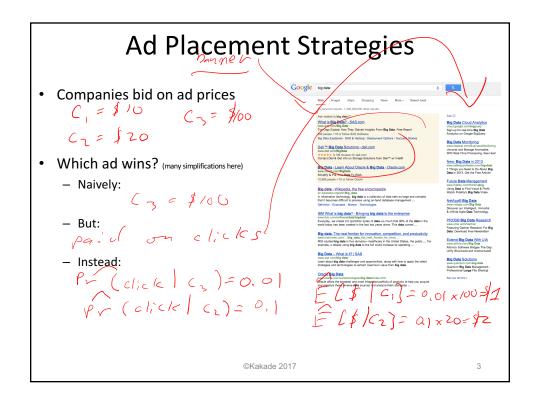
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#### **Announcements:**

- Lecture 2 cancelled
  - -TAs will hold a python recitation
- HW1 posted today.
- (starting NEXT week) TA office hours
- Readings: please do them.
- Project Proposals: please start thinking about it!
- Today:
  - Review: click prediction and logistic regression

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## Key Task: Estimating Click Probabilities

- What is the probability that user i will click on ad j
- Not important just for ads:
  - Optimize search results
  - Suggest news articles
  - Recommend products
- Methods much more general, useful for:
  - Classification
  - Regression
  - Density estimation

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## **Learning Problem for Click Prediction**

- Prediction task:  $\forall \in \{0,1\}$   $\forall r \in \{0,1\}$   $\forall r \in \{0,1\}$
- X = (festives of ad, features of person,

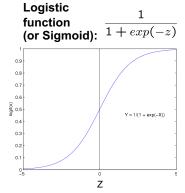
   Data: keymond, person index, the 
  { (xi, yi) }
- Many approaches (e.g., logistic regression, SVMs, naïve Bayes, decision trees, to show and, observe Y
  - Focus on logistic regression; captures main concepts, ideas generalize to other approaches

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## **Logistic Regression**

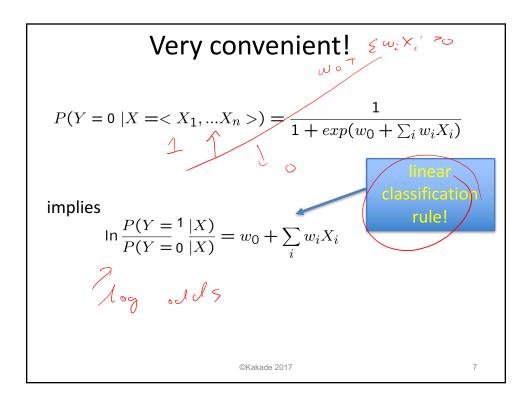
- Learn P(Y|X) directly
  - ☐ Assume a particular functional form
  - ☐ Sigmoid applied to a linear function of the data:

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



Features can be discrete or continuous!

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## Digression: Logistic regression more generally

Logistic regression in more general case, where Y in  $\{y_1,...,y_R\}$ 

for k<R

$$P(Y = y_k | X) = \frac{\exp(w_{k0} + \sum_{i=1}^{n} w_{ki} X_i)}{1 + \sum_{i=1}^{R-1} \exp(w_{i0} + \sum_{i=1}^{n} w_{ii} X_i)}$$

for k=R (normalization, so no weights for this class)

$$P(Y = y_R | X) = \frac{1}{1 + \sum_{j=1}^{R-1} \exp(w_{j0} + \sum_{i=1}^{n} w_{ji} X_i)}$$

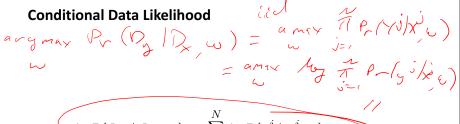
Features can be discrete or continuous!

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#### Loss function: Conditional Likelihood

• Have a bunch of iid data of the form:

• Discriminative (logistic regression) loss function:



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

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### Expressing Conditional Log Likelihood

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

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

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

$$= \sum_{j} \sqrt{|\mathbf{y}^{j}|} \ln P(Y = 1|\mathbf{x}^{j}, \mathbf{w}) + (1 - y^{j}) \ln P(Y = 0|\mathbf{x}^{j}, \mathbf{w})$$

$$= \sum_{j} \sqrt{|\mathbf{w}_{0}|} \left( \sum_{i=1}^{d} w_{i} x_{i}^{j} \right) - \ln \left( 1 + \exp(w_{0} + \sum_{i=1}^{d} w_{i} x_{i}^{j}) \right)$$

$$= \sum_{j} \sqrt{|\mathbf{w}_{0}|} \left( \sum_{i=1}^{d} w_{i} x_{i}^{j} \right) - \ln \left( 1 + \exp(w_{0} + \sum_{i=1}^{d} w_{i} x_{i}^{j}) \right)$$

## Maximizing Conditional Log Likelihood

$$l(\mathbf{w}) \equiv \ln \prod_{j} P(y^{j} | \mathbf{x}^{j}, \mathbf{w})$$

$$= \sum_{j} y^{j} (w_{0} + \sum_{i=1}^{d} w_{i} x_{i}^{j}) - \ln \left( 1 + \exp(w_{0} + \sum_{i=1}^{d} w_{i} x_{i}^{j}) \right)$$

Good news: *I*(**w**) is concave function of **w**, no local optima problems

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Bad news: no closed-form solution to maximize  $I(\mathbf{w})$ 

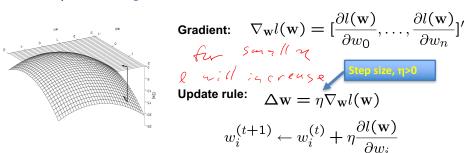
Good news: concave functions easy to optimize

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## Optimizing concave function – Gradient ascent

- Conditional likelihood for logistic regression is concave
- Find optimum with gradient ascent



- · Gradient ascent is simplest of optimization approaches
  - e.g., Conjugate gradient ascent much better (see reading)

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### **Gradient Ascent for LR**

Gradient ascent algorithm: iterate until change <  $\epsilon$ 

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

For 
$$i = 1,...,d$$
,

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

$$(y^j - \hat{Y}^j)$$

repeat

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## Regularized Conditional Log Likelihood

- If data are linearly separable, weights go to infinity
- 2 W 3
- Leads to overfitting → Penalize large weights
- Add regularization penalty, e.g., L<sub>2</sub>:

$$\ell(\mathbf{w}) = \ln \prod_{j} P(y^{j} | \mathbf{x}^{j}, \mathbf{w})) - \underbrace{\frac{\lambda}{2} ||\mathbf{w}||_{2}^{2}}$$

Practical note about w<sub>0</sub>:



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## Standard v. Regularized Updates

Maximum conditional likelihood estimate

$$\begin{aligned} \mathbf{w}^* &= \arg\max_{\mathbf{w}} \ln \left[ \prod_{j=1}^N P(y^j \mid \mathbf{x}^j, \mathbf{w}) \right] \\ w_i^{(t+1)} &\leftarrow w_i^{(t)} + \eta \sum_j x_i^j [y^j - \hat{P}(Y^j = \mathbf{1} \mid \mathbf{x}^j_{\text{(f)}} \mathbf{w})] \end{aligned}$$

Regularized maximum conditional likelihood estimate

$$\mathbf{w}^* = \arg \max_{\mathbf{w}} \ln \left[ \prod_{j} P(y^j | \mathbf{x}^j, \mathbf{w}) \right] - \frac{\lambda}{2} \sum_{i>0} w_i^2$$

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

## Stopping criterion / >>



$$\ell(\mathbf{w}) = \ln \prod_{j} P(y^{j} | \mathbf{x}^{j}, \mathbf{w})) - \frac{\lambda}{2} ||\mathbf{w}||_{2}^{2}$$

- Regularized logistic regression is strongly concave
  - Negative second derivative bounded away from zero:





- Strong concavity (convexity) is super helpful!!
- For example, for strongly concave *l*(**w**):

$$\ell(\mathbf{w}^*) - \ell(\mathbf{w}) \le \frac{1}{2\lambda} ||\nabla \ell(\mathbf{w})||_2^2$$

## Convergence rates for gradient descent/ascent

• Number of iterations to get to accuracy

$$\ell(\mathbf{w}^*) - \ell(\mathbf{w}) \le \epsilon$$

- If func I(w) Lipschitz:  $O(1/\epsilon^2)$
- If gradient of func Lipschitz:  $O(1/\epsilon)$
- If func is strongly convex:  $O(\ln(1/\epsilon))$

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## Challenge 1: Complexity of computing gradients

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

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

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## Challenge 2: Data is streaming

- Assumption thus far: Batch data
- But, click prediction is a streaming data task:
  - User enters query, and ad must be selected:
    - Observe x<sup>j</sup>, and must predict y<sup>j</sup>
  - User either clicks or doesn't click on ad:
    - Label y<sup>j</sup> is revealed afterwards
      - Google gets a reward if user clicks on ad
  - Weights must be updated for next time:

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## **Learning Problems as Expectations**

- Minimizing loss in training data:
  - Given dataset:
    - Sampled iid from some distribution  $p(\mathbf{x})$  on features:
  - Loss function, e.g., hinge loss, logistic loss,...
  - We often minimize loss in training data:

$$\ell_{\mathcal{D}}(\mathbf{w}) = \frac{1}{N} \sum_{j=1}^{N} \ell(\mathbf{w}, \mathbf{x}^{j})$$

• 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

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## **Gradient Ascent in Terms of Expectations**

• "True" objective function:

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

- Taking the gradient:
- "True" gradient ascent rule:
- How do we estimate expected gradient?

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

- "True" gradient:  $abla \ell(\mathbf{w}) = E_{\mathbf{x}} \left[ 
  abla \ell(\mathbf{w}, \mathbf{x}) \right]$
- Sample based approximation:
- What if we estimate gradient with just one sample???
  - Unbiased estimate of gradient
  - Very noisy!
  - Called stochastic gradient ascent (or descent)
    - Among many other names
  - VERY useful in practice!!!

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#### Stochastic Gradient Ascent: General Case

- Given a stochastic function of parameters:
  - Want to find maximum
- Start from **w**<sup>(0)</sup>
- · Repeat until convergence:
  - Get a sample data point x<sup>t</sup>
  - Update parameters:
- · Works in the online learning setting!
- · Complexity of each gradient step is constant in number of examples!
- In general, step size changes with iterations

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## Stochastic Gradient Ascent for Logistic Regression

• Logistic loss as a stochastic function:

$$E_{\mathbf{x}}\left[\ell(\mathbf{w}, \mathbf{x})\right] = E_{\mathbf{x}}\left[\ln P(y|\mathbf{x}, \mathbf{w}) - \frac{\lambda}{2}||\mathbf{w}||_{2}^{2}\right]$$

• Batch gradient ascent updates:

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

- Stochastic gradient ascent updates:
  - Online setting:

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

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## Convergence Rate of SGD

- Theorem:
  - (see Nemirovski et al '09 from readings)
  - Let f be a strongly convex stochastic function
  - Assume gradient of f is Lipschitz continuous and bounded
  - Then, for step sizes:
  - The expected loss decreases as O(1/t):

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## Convergence Rates for Gradient Descent/Ascent vs. SGD

· Number of Iterations to get to accuracy

$$\ell(\mathbf{w}^*) - \ell(\mathbf{w}) \le \epsilon$$

- · Gradient descent:
  - If func is strongly convex:  $O(\ln(1/\epsilon))$  iterations
- Stochastic gradient descent:
  - If func is strongly convex:  $O(1/\epsilon)$  iterations
- Seems exponentially worse, but much more subtle:
  - Total running time, e.g., for logistic regression:
    - · Gradient descent:
    - SGD:
    - SGD can win when we have a lot of data
  - See readings for more details

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### What you should know about

### Logistic Regression (LR) and Click Prediction

- Click prediction problem:
  - Estimate probability of clicking
  - Can be modeled as logistic regression
- Logistic regression model: Linear model
- Gradient ascent to optimize conditional likelihood
- Overfitting + regularization
- Regularized optimization
  - Convergence rates and stopping criterion
- Stochastic gradient ascent for large/streaming data
  - Convergence rates of SGD

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