Case Study 1: Estimating Click Probabilities

SGD cont'd
AdaGrad

Machine Learning for Big Data
CSE547/STAT548, University of Washington
Emily Fox
April 2nd, 2015

Learning Problem for Click Prediction

- Prediction task: $X \to \{0,1\}$ $P(\text{click}=1 \mid X)$
- Features: $X = $ (feats of page, ad, user)
- Data: (x^i, y^i) (webpage1, ad7, user25, time12) ← x^i; click = 1 ← y^i
  - Batch: Fixed dataset $(x^1,y^1) \dots (x^N,y^N)$
  - Online: data as a stream; user arrives at a page → x^t → predict $\hat{y}$ click? → observe y^t
- Many approaches (e.g., logistic regression, SVMs, naïve Bayes, decision trees, boosting,…)
  - Focus on logistic regression; captures main concepts, ideas generalize to other approaches

Standard v. Regularized Updates

- Maximum conditional likelihood estimate

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \ln \left[\prod_{j=1}^{N} P(y^j \mid \mathbf{x}^j, \mathbf{w}) \right]$$

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

- Regularized maximum conditional likelihood estimate

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

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

neg. derivative ← move towards 0

Challenge 1: Complexity of computing gradients

d features

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

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

for each i; cache; $O(d)$; $[w_1^{(t)} \ldots w_d^{(t)}]$; $O(Nd)$

$\forall$ features i, cost is $O(Nd^2)$ ... can cache $p(y^j=1|x^j, w^{(t)})$ → $O(Nd)$

In "big data" - N is very large

$O(Nd)$ for only taking little η step

Challenge 2: Data is streaming

- Assumption thus far: **Batch data** $\sum_{j=1}^{N} \ldots$
- But, click prediction is a streaming data task:
  - User enters query, and ad must be selected:
    - Observe $\mathbf{x}^j$, and must predict y^j

  (person) → (query) → x^j → predict $\hat{y}^j$ (click?) → show ad

  - User either clicks or doesn't click on ad:
    - Label y^j is revealed afterwards
      - Google gets a reward if user clicks on ad
  - Weights must be updated for next time:

  $w^{(t+1)} \leftarrow w^{(t)} + \Delta$ ← depends just on recent example(s)

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: $x^j \overset{iid}{\sim} p(x)$

$$\nabla \ell(w) = E_x[\nabla \ell(w,x)] \approx \hat{\nabla} \ell(w) = \frac{1}{N}\sum_{j=1}^{N} \nabla \ell(w, x^j)$$

the bigger N, the closer $\hat{\nabla}\ell$ to $\nabla \ell$

- What if we estimate gradient with just one sample??? $N=1$, $x^{(t)}$
  - Unbiased estimate of gradient: $\nabla \ell(w) \approx \hat{\nabla}\ell(w) = \nabla \ell(w, x^{(t)})$
    $E_x[\hat{\nabla}\ell(w)] = E_{x^{(t)}}[\nabla \ell(w, x^{(t)})] = \nabla \ell(w)$
  - Very noisy!
  - Called stochastic gradient ascent (or descent)
    - Among many other names
  - VERY useful in practice!!!

Stochastic Gradient Ascent: General Case

- Given a stochastic function of parameters:
  - Want to find maximum
- Start from $\mathbf{w}^{(0)}$
- Repeat until convergence:
  - Get a sample data point $\mathbf{x}^t$
  - 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

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:

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

Convergence Rate of SGD

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

Convergence Rates for Gradient Descent/Ascent vs. SGD

- Number of Iterations to get to accuracy

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

- Gradient descent:
  - If func is strongly convex: O(ln(1/ϵ)) iterations
- Stochastic gradient descent:
  - If func is strongly convex: O(1/ϵ) 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

Constrained SGD: Projected Gradient

- Consider an arbitrary restricted feature space $\mathbf{w} \in \mathcal{W}$
- Optimization objective:
- If $\mathbf{w} \in \mathcal{W}$, can use ***projected gradient*** for (sub)gradient descent

$\mathbf{w}^{(t+1)} =$

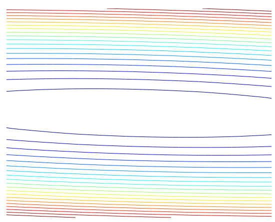
Motivating AdaGrad (Duchi, Hazan, Singer 2011)

- Assuming $\mathbf{w} \in \mathbb{R}^d$, standard stochastic (sub)gradient descent updates are of the form:

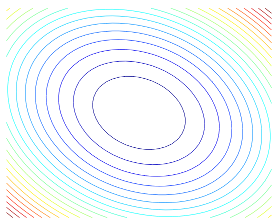
$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \eta_t g_{t,i}$$

- Should all features share the same learning rate?
- Often have high-dimensional feature spaces
  - Many features are irrelevant
  - Rare features are often very informative
- Adagrad provides a feature-specific adaptive learning rate by incorporating knowledge of the geometry of past observations

Why Adapt to Geometry?



Hard



Nice

y_t	$x_{t,1}$	$x_{t,2}$	$x_{t,3}$
1	1	0	0
-1	.5	0	1
1	-.5	1	0
-1	0	0	0
1	.5	0	0
-1	1	0	0
1	-1	1	0
-1	-.5	0	1

Examples from Duchi et al. ISMP 2012 slides

1. Frequent, irrelevant
2. Infrequent, predictive
3. Infrequent, predictive

Not All Features are Created Equal

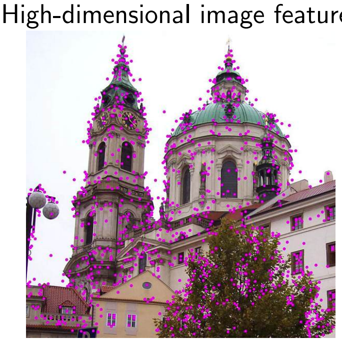
- Examples:

Text data:

```
 The most unsung birthday
in American business and
technological history
this year may be the 50th
anniversary of the Xerox
914 photocopier.ᵃ
```

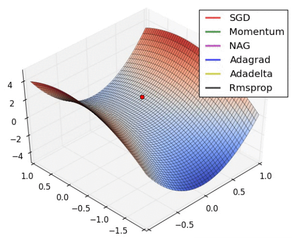
[a] *The Atlantic*, July/August 2010.

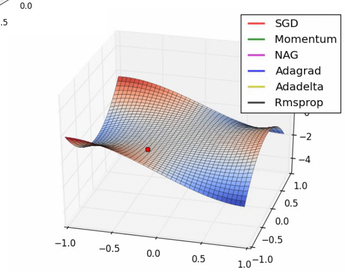
High-dimensional image features

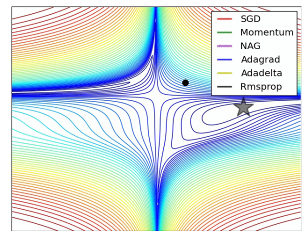


Images from Duchi et al. ISMP 2012 slides

Visualizing Effect







Credit:
http://imgur.com/a/Hqolp

Regret Minimization

- How do we assess the performance of an online algorithm?

- Algorithm iteratively predicts $\mathbf{w}^{(t)}$
- Incur ***loss*** $\ell_t(\mathbf{w}^{(t)})$
- ***Regret***:
  What is the total incurred loss of algorithm relative to the best choice of $\mathbf{w}$ that could have been made ***retrospectively***

$$R(T) = \sum_{t=1}^{T} \ell_t(\mathbf{w}^{(t)}) - \inf_{\mathbf{w} \in \mathcal{W}} \sum_{t=1}^{T} \ell_t(\mathbf{w})$$

Regret Bounds for Standard SGD

- Standard projected gradient stochastic updates:

$$\mathbf{w}^{(t+1)} = \arg\min_{\mathbf{w}\in\mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta g_t)||_2^2$$

- Standard regret bound:

$$\sum_{t=1}^{T} \ell_t(\mathbf{w}^{(t)}) - \ell_t(\mathbf{w}^*) \leq \frac{1}{2\eta}||\mathbf{w}^{(1)} - \mathbf{w}^*||_2^2 + \frac{\eta}{2}\sum_{t=1}^{T}||g_t||_2^2$$

Projected Gradient using Mahalanobis

- Standard projected gradient stochastic updates:

$$\mathbf{w}^{(t+1)} = \arg\min_{\mathbf{w}\in\mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta g_t)||_2^2$$

- What if instead of an L_2 metric for projection, we considered the ***Mahalanobis*** norm

$$\mathbf{w}^{(t+1)} = \arg\min_{\mathbf{w}\in\mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta A^{-1} g_t)||_A^2$$

Mahalanobis Regret Bounds

$$\mathbf{w}^{(t+1)} = \arg\min_{\mathbf{w}\in\mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta A^{-1} g_t)||_A^2$$

- **What *A* to choose?**
- Regret bound now:

$$\sum_{t=1}^{T} \ell_t(\mathbf{w}^{(t)}) - \ell_t(\mathbf{w}^*) \leq \frac{1}{2\eta}||\mathbf{w}^{(1)} - \mathbf{w}^*||_2^2 + \frac{\eta}{2}\sum_{t=1}^{T} ||g_t||_{A^{-1}}^2$$

- What if we minimize upper bound on regret w.r.t. *A* in hindsight?

$$\min_A \sum_{t=1}^{T} g_t^T A^{-1} g_t$$

Mahalanobis Regret Minimization

- Objective:

$$\min_A \sum_{t=1}^{T} g_t^T A^{-1} g_t \qquad \text{subject to } A \succeq 0, \mathrm{tr}(A) \leq C$$

- Solution:

$$A = c\left(\sum_{t=1}^{T} g_t g_t^T\right)^{\frac{1}{2}}$$

For proof, see Appendix E, Lemma 15 of Duchi et al. 2011.
Uses "trace trick" and Lagrangian.

- *A* defines the norm of the metric space we should be operating in

AdaGrad Algorithm

- At time *t*, estimate optimal (sub)gradient modification *A* by

$$A_t = \left(\sum_{\tau=1}^{t} g_\tau g_\tau^T \right)^{\frac{1}{2}}$$

- For *d* large, A_t is computationally intensive to compute. Instead,

- Then, algorithm is a simple modification of normal updates:

$$\mathbf{w}^{(t+1)} = \arg \min_{\mathbf{w} \in \mathcal{W}} ||\mathbf{w} - (\mathbf{w}^{(t)} - \eta \text{diag}(A_t)^{-1} g_t)||^2_{\text{diag}(A_t)}$$

AdaGrad in Euclidean Space

- For $\mathcal{W} = \mathbb{R}^d$,

- For each feature dimension,

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \eta_{t,i} g_{t,i}$$

where

$$\eta_{t,i} =$$

- That is,

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \frac{\eta}{\sqrt{\sum_{\tau=1}^{t} g_{\tau,i}^2}} g_{t,i}$$

- Each feature dimension has it's own learning rate!
  - Adapts with *t*
  - Takes geometry of the past observations into account
  - Primary role of η is determining rate the first time a feature is encountered

AdaGrad Theoretical Guarantees

- AdaGrad regret bound:

$$R_\infty := \max_t ||\mathbf{w}^{(t)} - \mathbf{w}^*||_\infty$$

$$\sum_{t=1}^{T} \ell_t(\mathbf{w}^{(t)}) - \ell_t(\mathbf{w}^*) \leq 2R_\infty \sum_{i=1}^{d} ||g_{1:T,i}||_2$$

  - In stochastic setting:

$$\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=1}^{T} w^{(t)}\right)\right] - \ell(\mathbf{w}^*) \leq \frac{2R_\infty}{T} \sum_{i=1}^{d} \mathbb{E}[||g_{1:T,j}||_2]$$

- This really is used in practice!
- Many cool examples. Let's just examine one…

AdaGrad Theoretical Example

- Expect to out-perform when gradient vectors are *sparse*
- SVM hinge loss example:

$$\ell_t(\mathbf{w}) = [1 - y^t \langle \mathbf{x}^t, \mathbf{w} \rangle]_+$$

$$\mathbf{x}^t \in \{-1, 0, 1\}^d$$

- If $x_j^t \neq 0$ with probability $\propto j^{-\alpha}, \quad \alpha > 1$

$$\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=1}^{T} \mathbf{w}^{(t)}\right)\right] - \ell(\mathbf{w}^*) = \mathcal{O}\left(\frac{||\mathbf{w}^*||_\infty}{\sqrt{T}} \cdot \max\{\log d, d^{1-\alpha/2}\}\right)$$

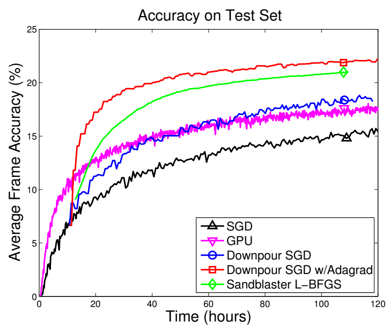
- Previously best known method: $\mathbb{E}\left[\ell\left(\frac{1}{T}\sum_{t=1}^{T} \mathbf{w}^{(t)}\right)\right] - \ell(\mathbf{w}^*) = \mathcal{O}\left(\frac{||\mathbf{w}^*||_\infty}{\sqrt{T}} \cdot \sqrt{d}\right)$

Neural Network Learning

- Very non-convex problem, but use SGD methods anyway

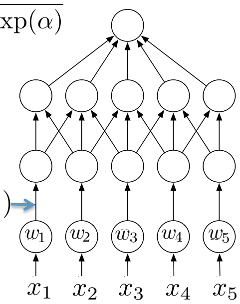
$$\ell(w, x) = \log(1 + \exp(\langle [p(\langle w_1, x_1 \rangle) \cdots p(\langle w_k, x_k \rangle)], x_0 \rangle))$$

$$p(\alpha) = \frac{1}{1 + \exp(\alpha)}$$



(Dean et al. 2012)

$p(\langle w_1, x_1 \rangle)$



Distributed, $d = 1.7 \cdot 10^9$ parameters. SGD and AdaGrad use 80 machines (1000 cores), L-BFGS uses 800 (10000 cores)

Images from Duchi et al. ISMP 2012 slides

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
- AdaGrad motivation, derivation, and algorithm