Stochastic Gradient Descent

Machine Learning – CSE546

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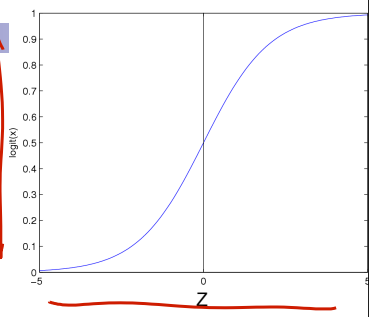
October 14, 2014

Logistic Regression

Logistic function (or Sigmoid): $\frac{1}{1+exp(-z)}$



- Learn P(Y|**X**) directly
  - Assume a particular functional form for link function
  - Sigmoid applied to a linear function of the input features: [0,1]

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

[0,1]

$w_0+\sum_i w_i X_i \in \mathbb{R}$

$z \in \mathbb{R}$

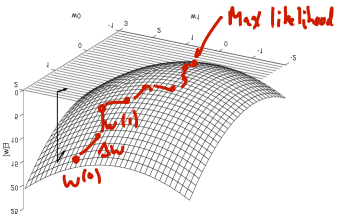
$$P(Y=1|X,w) = 1 - P(Y=0|X,w) = \frac{e^{w_0+\sum_i w_i X_i}}{1+e^{w_0+\sum_i w_i X_i}} \leftarrow h_i(X)$$

X_i indicators: $X_i = \mathbb{1}(\text{country} = \text{USA})$

Features can be discrete or continuous!

Optimizing concave function – Gradient ascent

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



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

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

Step size, $\eta > 0$

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

(choice of η? from theory $\eta = \frac{\alpha}{\sqrt{t}}$ or $\eta = \frac{\alpha}{t}$ or $\eta = \alpha$ for HW)

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

Newton, LBFGS, ...

Gradient Ascent for LR

initialize $w^{(0)} = 0$ or something else → all converge to same place, concavity

Gradient ascent algorithm: iterate until change < ε

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

small step — gradient direction

For i=1,…,k,

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

repeat

The Cost, The Cost!!! Think about the cost…

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

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

Learning Problems as Expectations

- Minimizing loss in training data:
  - Given dataset:
    - Sampled iid from some distribution p(**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

Gradient descent 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 descent rule:
- How do we estimate expected gradient?

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:
- 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!!!

Stochastic Gradient Ascent for Logistic Regression

- Logistic loss as a stochastic function:

$$E_{\mathbf{x}}\left[\ell(\mathbf{w},\mathbf{x})\right] = E_{\mathbf{x}}\left[\ln P(y|\mathbf{x},\mathbf{w}) - \lambda||\mathbf{w}||_2^2\right]$$

- 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:

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

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

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

Boosting

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Fighting the bias-variance tradeoff

- **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…**

Voting (Ensemble Methods)

- Instead of learning a single (weak) classifier, learn **many weak classifiers** that are **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!

- **But how do you ???**
  - force classifiers to learn about different parts of the input space?
  - weigh the votes of different classifiers?

Boosting [Schapire, 1989]

- Idea: given a weak learning alg, run it multiple times on (reweighted) training data, then let learned classifiers vote
- On each iteration *t*:
  - weight each training example by how incorrectly it was classified
  - Learn a hypothesis – h_t
  - A strength for this hypothesis – α_t
- Final classifier:
- **Practically useful**
- **Theoretically interesting**

Learning from weighted data

- **Sometimes not all data points are equal**
  - Some data points are more equal than others
- **Consider a weighted dataset**
  - D(j) – weight of *j* th training example ($\mathbf{x}^j$,y^j)
  - Interpretations:
    - *j* th training example counts as D(j) examples
    - If I were to "resample" data, I would get more samples of "heavier" data points
- **Now, in all calculations, whenever used, *j* th training example counts as D(j) "examples"**

AdaBoost

- Initialize weights to uniform dist: $D_1(j) = 1/N$
- For t = 1…T
  - Train weak learner h_t on distribution D_t over the data
  - Choose weight α_t
  - Update weights:

$$D_{t+1}(j) = \frac{D_t(j)\exp(-\alpha_t y^j h_t(x^j))}{Z_t}$$

    - Where Z_t is normalizer:

$$Z_t = \sum_{j=1}^{N} D_t(j)\exp(-\alpha_t y^j h_t(x^j))$$

- Output final classifier:

Picking Weight of Weak Learner

- Weigh h_t higher if it did well on training data (weighted by D_t):

$$\alpha_t = \frac{1}{2}\ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$$

  - Where ε_t is the weighted training error:

$$\epsilon_t = \sum_{j=1}^{N} D_t(j)\mathbb{1}[h_t(x^j) \neq y^j]$$

Why choose α_t for hypothesis h_t this way?

[Schapire, 1989]

Training error of final classifier is bounded by:

$$\frac{1}{N}\sum_{j=1}^{N}\mathbb{1}[H(x^j)\neq y^j] \leq \frac{1}{N}\sum_{j=1}^{N}\exp(-y^j f(x^j))$$

Where $f(x)=\sum_t \alpha_t h_t(x); H(x)=sign(f(x))$

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Where $f(x) = \sum_t \alpha_t h_t(x); H(x) = sign(f(x))$

If we minimize $\prod_t Z_t$, we minimize our training error

AdaBoost tightens this bound greedily, by choosing α_t and h_t on each iteration to minimize Z_t.

$$Z_t = \sum_{j=1}^{N} D_t(j)\exp(-\alpha_t y^j h_t(x^j))$$

Why choose α_t for hypothesis h_t this way?

[Schapire, 1989]

We can minimize this bound by choosing α_t on each iteration to minimize Z_t.

$$Z_t = \sum_{j=1}^{N} D_t(j)\exp(-\alpha_t y^j h_t(x^j))$$

For boolean target function, this is accomplished by [Freund & Schapire '97]:

$$\alpha_t = \tfrac{1}{2}\ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$$

You'll prove this in your homework! ☺

Strong, weak classifiers

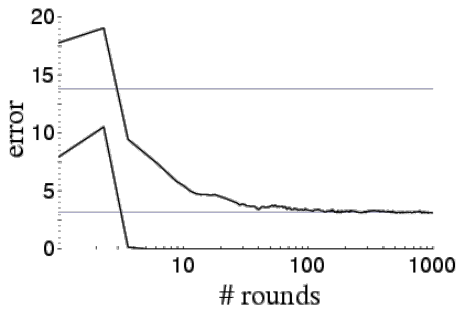
- If each classifier is (at least slightly) better than random
  - $\varepsilon_t < 0.5$
- AdaBoost will achieve zero *training error* (exponentially fast):

$$\frac{1}{N}\sum_{j=1}^{N}\mathbb{1}[H(x^j)\neq y^j] \leq \prod_{t=1}^{T} Z_t \leq \exp\left(-2\sum_{t=1}^{T}(1/2-\epsilon_t)^2\right)$$

- Is it hard to achieve better than random guessing?

Boosting results – Digit recognition

[Schapire, 1989]

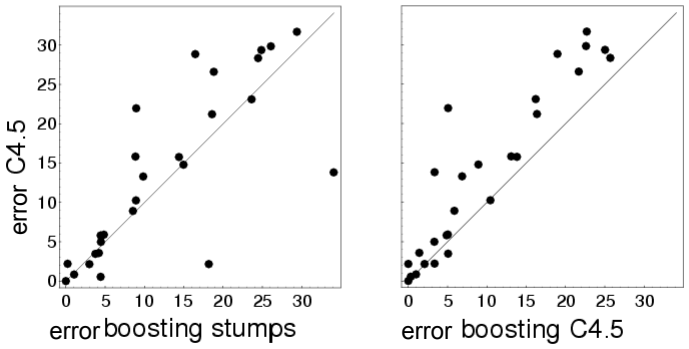


- Boosting often
  - Robust to overfitting
  - Test set error decreases even after training error is zero

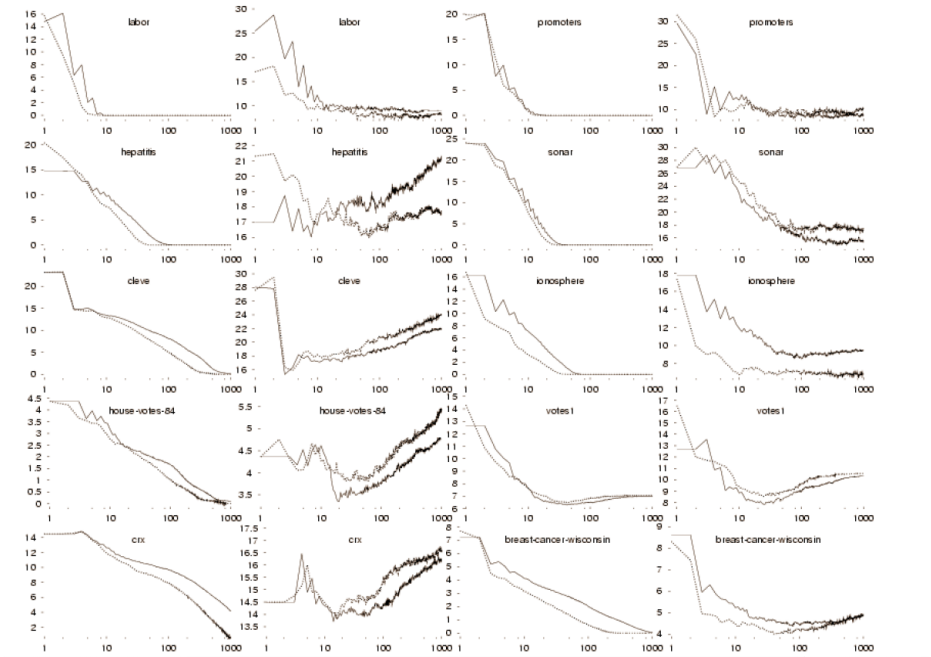
Boosting: Experimental Results

[Freund & Schapire, 1996]

Comparison of C4.5, Boosting C4.5, Boosting decision stumps (depth 1 trees), 27 benchmark datasets



AdaBoost and AdaBoost.MH on Train (left) and Test (right) data from Irvine repository. [Schapire and Singer, ML 1999]



Boosting and Logistic Regression

Logistic regression assumes:

$$P(Y = 1|X) = \frac{1}{1 + \exp(f(x))}$$

And tries to maximize data likelihood:

$$P(\mathcal{D}|H) = \prod_{j=1}^{N} \frac{1}{1 + \exp(-y^j f(x^j))}$$

Equivalent to minimizing log loss

$$\sum_{j=1}^{N} \ln(1 + \exp(-y^j f(x^j)))$$

Boosting and Logistic Regression

Logistic regression equivalent to minimizing log loss

$$\sum_{j=1}^{N} \ln(1 + \exp(-y^j f(x^j)))$$

Boosting minimizes similar loss function!!

$$\frac{1}{N} \sum_{j=1}^{N} \exp(-y^j f(x^j)) = \prod_{t=1}^{T} Z_t$$

Both smooth approximations of 0/1 loss!

Logistic regression and Boosting

Logistic regression:

- Minimize loss fn

$$\sum_{j=1}^{N} \ln(1 + \exp(-y^j f(x^j)))$$

- Define

$$f(x) = w_0 + \sum_i w_i x_i$$

where features x_i are predefined

- Weights w_i are learned in joint optimization

Boosting:

- Minimize loss fn

$$\sum_{j=1}^{N} \exp(-y^j f(x^j))$$

- Define

$$f(x) = \sum_t \alpha_t h_t(x)$$

where $h_t(x)$ defined dynamically to fit data

(not a linear classifier)

- Weights α_t learned incrementally

What you need to know about Boosting

- Combine weak classifiers to obtain very strong classifier
  - Weak classifier – slightly better than random on training data
  - Resulting very strong classifier – can eventually provide zero training error
- AdaBoost algorithm
- Boosting v. Logistic Regression
  - Similar loss functions
  - Single optimization (LR) v. Incrementally improving classification (B)
- Most popular application of Boosting:
  - Boosted decision stumps!
  - Very simple to implement, very effective classifier