## Ensemble learning Lecture 12

David Sontag New York University

Slides adapted from Luke Zettlemoyer, Vibhav Gogate, Rob Schapire, and Tommi Jaakkola

## **Ensemble methods**

### Machine learning competition with a \$1 million prize

#### Leaderboard Display top 20 💌 leaders. Team Name Rank Best Score % Improvement Last Submit Time 0.8553 10.10 2009-07-26 18:38:22 The Ensemble 10.09 2009-07-26 18:18:28 Grand Prize - RMSE <= 0.8563 3 Grand Prize Team 0.8571 9.91 2009-07-24 13:07:49 Opera Solutions and Vandelay United 0.8573 9.89 2009-07-25 20:05:52 4 5 Vandelay Industries ! 0.8579 9.83 2009-07-26 02:49:53 6 **PragmaticTheory** 0.8582 9.80 2009-07-12 15:09:53 7 BellKor in BigChaos 0.8590 9.71 2009-07-26 12:57:25 8 Dace 0.8603 9.58 2009-07-24 17:18:43 9 0.8611 2009-07-26 18:02:08 Opera Solutions 9.49 10 BellKor 0.8612 9.48 2009-07-26 17:19:11 9.47 2009-06-23 23:06:52 11 0.8613 **BigChaos** 12 Feeds2 0.8613 9.47 2009-07-24 20:06:46 Progress Prize 2008 - RMSE = 0.8616 - Winning Team: BellKor in BigChaos 0.8633 2009-07-21 02:04:40 13 9.26 xiangliang 14 0.8634 9.25 2009-07-26 15:58:34 Gravity 15 Ces 0.8642 9.17 2009-07-25 17:42:38 2009-07-20 03:26:12 16 Invisible Ideas 0.8644 9.14 17 0.8650 9.08 2009-07-22 14:10:42 Just a quy in a garage 18 0.8656 9.02 2009-07-25 16:00:54 Craig Carmichael 19 0.8658 9.00 2009-03-11 09:41:54 J Dennis Su 20 acmehill 0.8659 8.99 2009-04-16 06:29:35 Progress Prize 2007 - RMSE = 0.8712 - Winning Team: KorBell Cinematch score on guiz subset - RMSE = 0.9514



## **Bias/Variance Tradeoff**



Hastie, Tibshirani, Friedman "Elements of Statistical Learning" 2001

## Reduce Variance Without Increasing Bias

• Averaging reduces variance:

$$Var(\overline{X}) \quad \frac{Var(X)}{N}$$
 (when predictions are **independent**)

Average models to reduce model variance

One problem:

only one training set

where do multiple models come from?

## Bagging: Bootstrap Aggregation

- Leo Breiman (1994)
- Take repeated **bootstrap** samples from training set *D*.
- Bootstrap sampling: Given set D containing N training examples, create D' by drawing N examples at random with replacement from D.
- Bagging:
  - Create k bootstrap samples  $D_1 \dots D_k$ .
  - Train distinct classifier on each  $D_i$ .
  - Classify new instance by majority vote / average.

## Bagging

• Best case:  $Var(Bagging(L(x, D))) = \frac{Variance(L(x, D))}{N}$ 

In practice:

models are correlated, so reduction is smaller than 1/N variance of models trained on fewer training cases usually somewhat larger

Bagging Example



\_decision tree learning algorithm; very similar to ID3

# CART decision boundary



## 100 bagged trees



shades of blue/red indicate strength of vote for particular classification

## Reduce Bias<sup>2</sup> and Decrease Variance?

- Bagging reduces variance by averaging
- Bagging has little effect on bias
- Can we average *and* reduce bias?
- Yes:



#### Theory and Applications of Boosting

**Rob Schapire** 

#### Example: "How May I Help You?"

[Gorin et al.]

- goal: automatically categorize type of call requested by phone customer (Collect, CallingCard, PersonToPerson, etc.)
  - yes I'd like to place a collect call long distance please (Collect)
  - operator I need to make a call but I need to bill it to my office (ThirdNumber)
  - yes I'd like to place a call on my master card please (CallingCard)
  - I just called a number in sioux city and I musta rang the wrong number because I got the wrong party and I would like to have that taken off of my bill (BillingCredit)
- observation:
  - easy to find "rules of thumb" that are "often" correct
    - e.g.: "IF 'card' occurs in utterance THEN predict 'CallingCard' "
  - hard to find single highly accurate prediction rule

#### The Boosting Approach

- devise computer program for deriving rough rules of thumb
- apply procedure to subset of examples
- obtain rule of thumb
- apply to 2nd subset of examples
- obtain 2nd rule of thumb
- repeat T times

#### Key Details

- how to choose examples on each round?
  - concentrate on "hardest" examples (those most often misclassified by previous rules of thumb)
- how to combine rules of thumb into single prediction rule?
  - take (weighted) majority vote of rules of thumb

#### Boosting

- boosting = general method of converting rough rules of thumb into highly accurate prediction rule
- technically:
  - assume given "weak" learning algorithm that can consistently find classifiers ("rules of thumb") at least slightly better than random, say, accuracy ≥ 55% (in two-class setting) ["weak learning assumption"]
  - given sufficient data, a boosting algorithm can provably construct single classifier with very high accuracy, say, 99%

Preamble: Early History

#### Strong and Weak Learnability

- boosting's roots are in "PAC" learning model [Valiant '84]
- get random examples from unknown, arbitrary distribution
- strong PAC learning algorithm:
  - for any distribution with high probability given polynomially many examples (and polynomial time) can find classifier with arbitrarily small generalization error
- weak PAC learning algorithm
  - same, but generalization error only needs to be slightly better than random guessing  $(\frac{1}{2} \gamma)$
- [Kearns & Valiant '88]:
  - does weak learnability imply strong learnability?

#### If Boosting Possible, Then...

- can use (fairly) wild guesses to produce highly accurate predictions
- if can learn "part way" then can learn "all the way"
- should be able to improve any learning algorithm
- for any learning problem:
  - either can always learn with nearly perfect accuracy
  - or there exist cases where cannot learn even slightly better than random guessing

#### First Boosting Algorithms

- [Schapire '89]:
  - first provable boosting algorithm
- [Freund '90]:
  - "optimal" algorithm that "boosts by majority"
- [Drucker, Schapire & Simard '92]:
  - first experiments using boosting
  - limited by practical drawbacks
- [Freund & Schapire '95]:
  - introduced "AdaBoost" algorithm
  - strong practical advantages over previous boosting algorithms

#### Application: Detecting Faces

[Viola & Jones]

- problem: find faces in photograph or movie
- weak classifiers: detect light/dark rectangles in image



many clever tricks to make extremely fast and accurate

#### Basic Algorithm and Core Theory

- introduction to AdaBoost
- analysis of training error
- analysis of test error and the margins theory
- experiments and applications

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#### A Formal Description of Boosting

- given training set  $(x_1, y_1), \ldots, (x_m, y_m)$
- $y_i \in \{-1, +1\}$  correct label of instance  $x_i \in X$
- for t = 1, ..., T:
  - construct distribution  $D_t$  on  $\{1, \ldots, m\}$
  - find weak classifier ("rule of thumb")

 $h_t:X\to\{-1,+1\}$ 

with error  $\epsilon_t$  on  $D_t$ :

 $\epsilon_t = \Pr_{i \sim D_t}[h_t(x_i) \neq y_i]$ 

output final/combined classifier H<sub>final</sub>

#### AdaBoost

#### [with Freund]

- constructing  $D_t$ :
  - $D_1(i) = 1/m$
  - given  $D_t$  and  $h_t$ :

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if } y_i \neq h_t(x_i) \end{cases}$$
$$= \frac{D_t(i)}{Z_t} \exp(-\alpha_t y_i h_t(x_i))$$

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where  $Z_t = \text{normalization factor}$  $\alpha_t = \frac{1}{2} \ln \left( \frac{1 - \epsilon_t}{\epsilon_t} \right) > 0$ 

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• final classifier:

• 
$$H_{\text{final}}(x) = \operatorname{sign}\left(\sum_{t} \alpha_t h_t(x)\right)$$

#### Toy Example



weak classifiers = vertical or horizontal half-planes

Round 1



$$\epsilon_1 = 0.30$$
  
 $\alpha_1 = 0.42$ 

Round 2



Round 3



 ${}^{\epsilon_3=0.14}_{\alpha_3=0.92}$ 

#### **Final Classifier**





### **Voted combination of classifiers**

- The general problem here is to try to combine many simple "weak" classifiers into a single "strong" classifier
- $\bullet$  We consider voted combinations of simple binary  $\pm 1$  component classifiers

$$h_m(\mathbf{x}) = \alpha_1 h(\mathbf{x}; \theta_1) + \ldots + \alpha_m h(\mathbf{x}; \theta_m)$$

where the (non-negative) votes  $\alpha_i$  can be used to emphasize component classifiers that are more reliable than others



### **Components: decision stumps**

• Consider the following simple family of component classifiers generating  $\pm 1$  labels:

$$h(\mathbf{x}; \theta) = \operatorname{sign}(w_1 x_k - w_0)$$

where  $\theta = \{k, w_1, w_0\}$ . These are called *decision stumps*.

 Each decision stump pays attention to only a single component of the input vector





### Voted combination cont'd

• We need to define a loss function for the combination so we can determine which new component  $h(\mathbf{x}; \theta)$  to add and how many votes it should receive

$$h_m(\mathbf{x}) = \alpha_1 h(\mathbf{x}; \theta_1) + \ldots + \alpha_m h(\mathbf{x}; \theta_m)$$

• While there are many options for the loss function we consider here only a simple exponential loss

 $\exp\{-y\,h_m(\mathbf{x})\,\}$ 



## Modularity, errors, and loss

• Consider adding the  $m^{th}$  component:

$$\sum_{i=1}^{n} \exp\{-y_i[h_{m-1}(\mathbf{x}_i) + \alpha_m h(\mathbf{x}_i; \theta_m)]\}$$
$$= \sum_{i=1}^{n} \exp\{-y_i h_{m-1}(\mathbf{x}_i) - y_i \alpha_m h(\mathbf{x}_i; \theta_m)\}$$



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$$= \sum_{i=1}^{n} \underbrace{\exp\{-y_i h_{m-1}(\mathbf{x}_i)\}}_{\text{fixed at stage } m} \exp\{-y_i \alpha_m h(\mathbf{x}_i; \theta_m)\}$$

## Modularity, errors, and loss

• Consider adding the  $m^{th}$  component:

$$\sum_{i=1}^{n} \exp\{-y_{i}[h_{m-1}(\mathbf{x}_{i}) + \alpha_{m}h(\mathbf{x}_{i};\theta_{m})]\}$$

$$= \sum_{i=1}^{n} \exp\{-y_{i}h_{m-1}(\mathbf{x}_{i}) - y_{i}\alpha_{m}h(\mathbf{x}_{i};\theta_{m})\}$$

$$= \sum_{i=1}^{n} \underbrace{\exp\{-y_{i}h_{m-1}(\mathbf{x}_{i})\}}_{\text{fixed at stage }m} \exp\{-y_{i}\alpha_{m}h(\mathbf{x}_{i};\theta_{m})\}$$

$$= \sum_{i=1}^{n} W_{i}^{(m-1)} \exp\{-y_{i}\alpha_{m}h(\mathbf{x}_{i};\theta_{m})\}$$

So at the  $m^{th}$  iteration the new component (and the votes) should optimize a weighted loss (weighted towards mistakes).

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### Empirical exponential loss cont'd

- To increase modularity we'd like to further decouple the optimization of  $h(\mathbf{x}; \theta_m)$  from the associated votes  $\alpha_m$
- To this end we select  $h(\mathbf{x}; \theta_m)$  that optimizes the rate at which the loss would decrease as a function of  $\alpha_m$

$$\frac{\partial}{\partial \alpha_m}\Big|_{\alpha_m=0} \sum_{i=1}^n W_i^{(m-1)} \exp\{-y_i \alpha_m h(\mathbf{x}_i; \theta_m)\} = \left[\sum_{i=1}^n W_i^{(m-1)} \exp\{-y_i \alpha_m h(\mathbf{x}_i; \theta_m)\} \cdot \left(-y_i h(\mathbf{x}_i; \theta_m)\right)\right]_{\alpha_m=0} = \left[\sum_{i=1}^n W_i^{(m-1)} \left(-y_i h(\mathbf{x}_i; \theta_m)\right)\right]$$



### Empirical exponential loss cont'd

• We find  $h(\mathbf{x}; \hat{\theta}_m)$  that minimizes

$$-\sum_{i=1}^{n} W_i^{(m-1)} y_i h(\mathbf{x}_i; \theta_m)$$

We can also normalize the weights:

$$\begin{split} & -\sum_{i=1}^{n} \frac{W_{i}^{(m-1)}}{\sum_{j=1}^{n} W_{j}^{(m-1)}} y_{i} h(\mathbf{x}_{i}; \theta_{m}) \\ & = -\sum_{i=1}^{n} \tilde{W}_{i}^{(m-1)} y_{i} h(\mathbf{x}_{i}; \theta_{m}) \end{split}$$
  
so that  $\sum_{i=1}^{n} \tilde{W}_{i}^{(m-1)} = 1.$ 

### Selecting a new component: summary

• We find  $h(\mathbf{x}; \hat{\theta}_m)$  that minimizes

$$-\sum_{i=1}^{n} \tilde{W}_{i}^{(m-1)} y_{i} h(\mathbf{x}_{i}; \theta_{m})$$

where 
$$\sum_{i=1}^{n} \tilde{W}_i^{(m-1)} = 1$$
.

•  $\alpha_m$  is subsequently chosen to minimize

$$\sum_{i=1}^{n} \tilde{W}_{i}^{(m-1)} \exp\{-y_{i}\alpha_{m}h(\mathbf{x}_{i};\hat{\theta}_{m})\}$$



### The AdaBoost algorithm

- **0)** Set  $\tilde{W}_{i}^{(0)} = 1/n$  for i = 1, ..., n
- 1) At the  $m^{th}$  iteration we find (any) classifier  $h(\mathbf{x}; \hat{\theta}_m)$  for which the weighted classification error  $\epsilon_m$

$$\epsilon_m = 0.5 - \frac{1}{2} \left( \sum_{i=1}^n \tilde{W}_i^{(m-1)} y_i h(\mathbf{x}_i; \hat{\theta}_m) \right)$$

is better than chance.

2) The new component is assigned votes based on its error:

$$\hat{\alpha}_m = 0.5 \log((1 - \epsilon_m)/\epsilon_m)$$

**3)** The weights are updated according to  $(Z_m \text{ is chosen so that the new weights } \tilde{W}_i^{(m)} \text{ sum to one})$ :

$$\tilde{W}_i^{(m)} = \frac{1}{Z_m} \cdot \tilde{W}_i^{(m-1)} \cdot \exp\{-y_i \hat{\alpha}_m h(\mathbf{x}_i; \hat{\theta}_m)\}$$