Boosting

Machine Learning - 10601

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[partly based on slides of Rob Schapire and Carlos Guestrin]

http://www.cs.cmu.edu/~ggordon/10601/

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Ensembles of trees

BAGGING and RANDOM FORESTS

- learn many **big trees**
- each tree aims to fit the **same target concept**
  – random training sets
  – randomized tree growth
- voting ≈ averaging: **DECREASE in VARIANCE**

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BOOSTING

- learn many **small trees** (**weak** classifiers)
- each tree 'specializes' to a **different part** of target concept
  - reweight training examples
  - higher weights where still errors
- voting increases expressivity: **DECREASE in BIAS**

Boosting

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  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)
  - given sufficient data, a boosting algorithm can provably construct **single classifier** with **very high accuracy**, say, **99%**

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 $x_i \in X$

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  - construct distribution D_t on $\{1, \ldots, m\}$

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  - find weak classifier ("rule of thumb")

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

    with small error ϵ_t on D_t:

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

WEIGHTED ERROR

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- output final classifier H_{final}

AdaBoost

[Freund-Schapire 1995]

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  - $D_1(i) = 1/m$

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  - given D_t and h_t:

GOT RIGHT

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

GOT WRONG

$\alpha_t > 0$

AdaBoost

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$\in \{-1, +1\}$

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$$= \frac{D_t(i)}{Z_t} \exp(-\alpha_t \, y_i \, h_t(x_i))$$

where Z_t = normalization constant

$$\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right) > 0$$

LARGER IF h_t MORE RIGHT

$\frac{\text{WEIGHT RIGHT}}{\text{WEIGHT WRONG}}$

WEIGHTED ERROR OF h_t

according to D_t

AdaBoost

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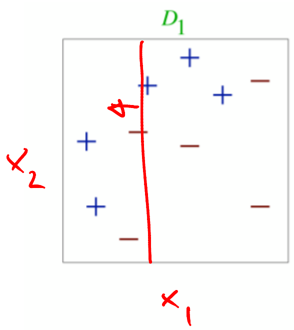
- final classifier:
  - $H_{\text{final}}(x) = \text{sign}\left(\sum_t \alpha_t h_t(x) \right)$

LARGER IF h_t MORE RIGHT

Toy example

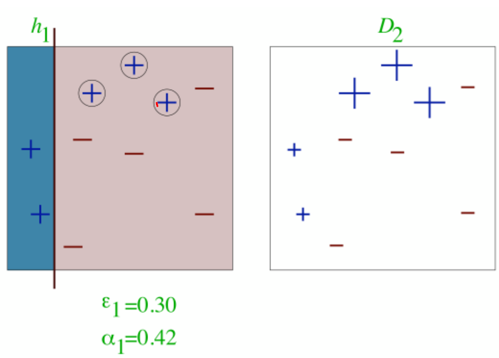


$x_1 < c_1$

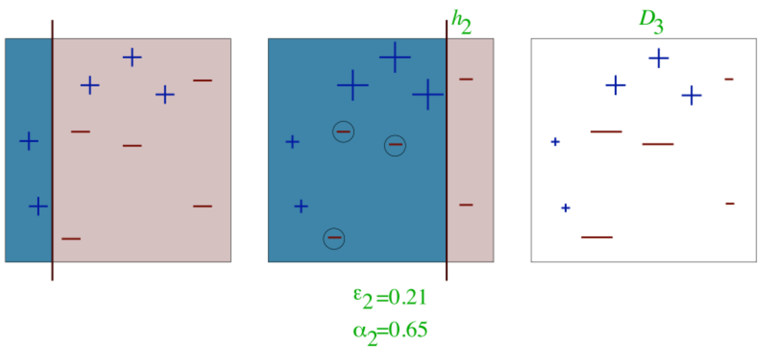
\+ −

weak classifiers = decision stumps
(vertical or horizontal half-planes)

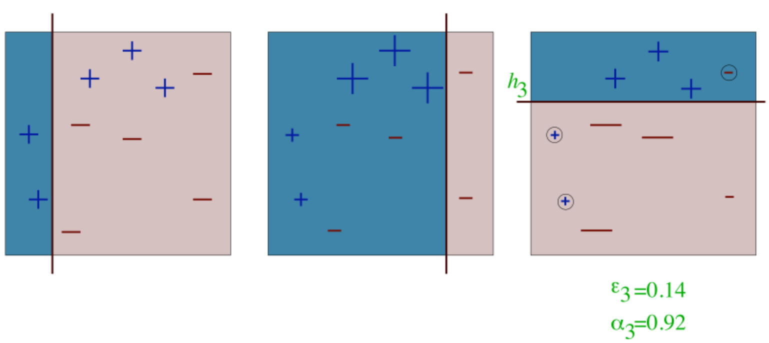
Round 1



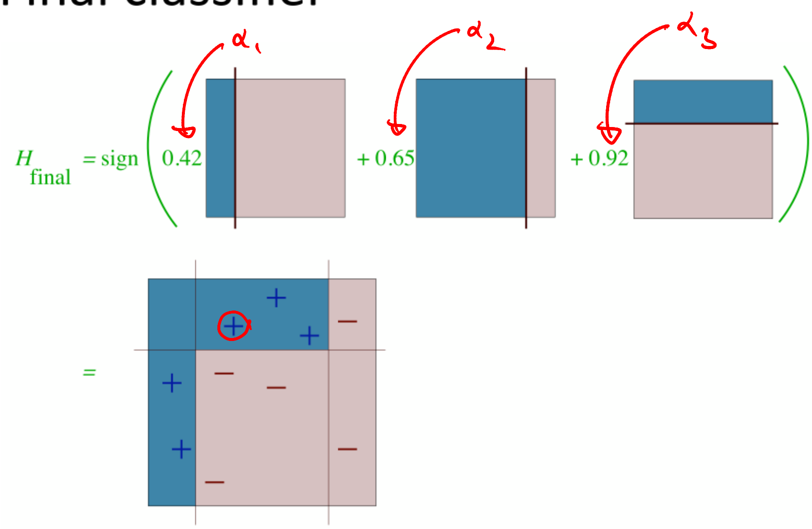
Round 2



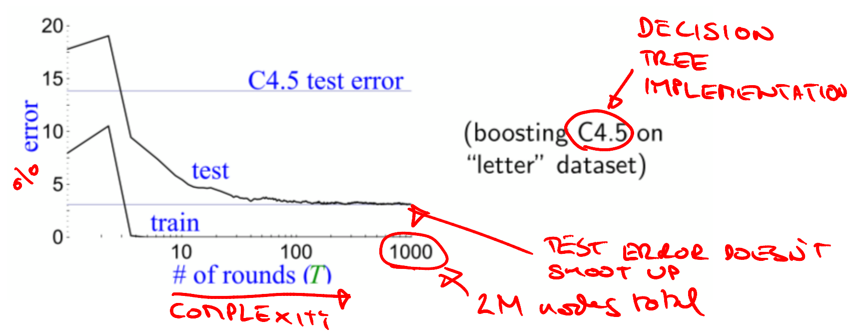
Round 3



Final classifier



A typical run of AdaBoost



- training error rapidly drops
  (combining weak learners increases expressivity)
- test error does not increase with number of trees T
  (robustness to overfitting)

Bounding *training* error

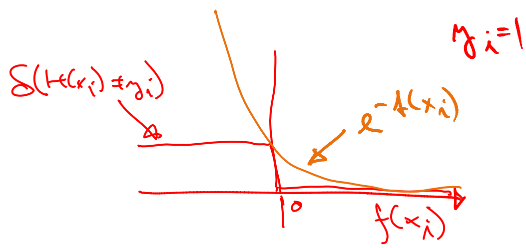
Training error of final classifier is bounded by:

INDICATOR

CURRENT WEIGHTED f VOTE

$$\text{err}_{\text{train}}(H) = \frac{1}{m}\sum_{i=1}^{m} \delta(H(x_i) \neq y_i) \leq \frac{1}{m}\sum_{i=1}^{m} \exp(-y_i f(x_i))$$

where $f(x) = \sum_{t=1}^{T} \alpha_t h_t(x)$; $H(x) = \text{sign}(f(x))$.



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Last step can be proved by unraveling the definition of $D_t(i)$:

$$D_{t+1}(i) = \frac{D_t(i)\exp(-y_i \alpha_t h_t(x_i))}{Z_t}$$

$$D_{T+1}(i) = \frac{1}{m}\frac{\exp(-y_i f(x_i))}{\prod_{t=1}^{T} Z_t}$$

Optimizing α_t

By minimizing $\prod_t Z_t$, we minimize the training error.

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We can tighten this bound greedily, by choosing α_t on each round to minimize Z_t:

$$Z_t = \sum_{i=1}^{m} D_t(i) \underbrace{\exp(-y_i \alpha_t h_t(x_i))}_{\text{WEIGHT UPDATE}}$$

OLD DIST.

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Since $h_t(x_i) \in \{-1, 1\}$, we can find this explicitly:

$$Z_t = w_t^{\text{CORRECT}} \cdot e^{-\alpha_t} + w_t^{\text{WRONG}} \cdot e^{\alpha_t} \quad x$$

$1/x$

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$w_t^{CORRECT}$

w_t^{WRONG}

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Intuition: In each round, we adjust example weights, so that the accuracy of the last rule of thumb h_t drops to 50%.

Weak learners to Strong learners

Plugging the optimal α_t in the error bound:

$$\frac{1}{m}\sum_{i=1}^{m}\delta(H(x_i)\neq y_i)\leq\prod_{t=1}^{T}Z_t$$

Weak learners to Strong learners

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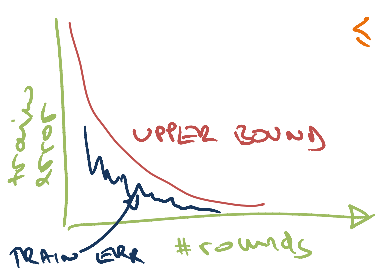
$$\frac{1}{m}\sum_{i=1}^{m}\delta(H(x_i)\neq y_i)\leq\prod_{t=1}^{T}Z_t\leq\exp\Big(-2\sum_{t=1}^{T}\underbrace{(0.5-\epsilon_t)^2}_{(0.05)^2}\Big)$$

$\leq \exp(-2 T\, 0.05^2)$



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Now, if each rule of thumb (at least slightly) better than random:

$\epsilon_t \leq 0.5 - \gamma$ for $\gamma > 0$

then training error drops exponentially fast:

$$\frac{1}{m}\sum_{i=1}^{m}\delta(H(x_i)\neq y_i) \leq \prod_{t=1}^{T} Z_t \leq \exp\left(-2\sum_{t=1}^{T}(0.5-\epsilon_t)^2\right) \leq e^{-2T\gamma^2}$$

Bounding *true* error

[Freund-Schapire 1997]

$e^{-2T\gamma^2}$

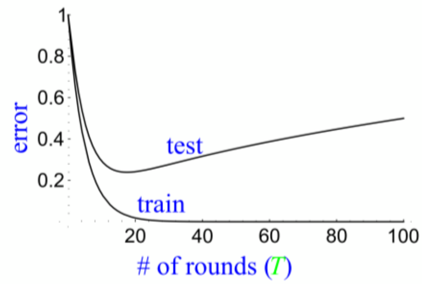
PENALTY FOR COMPLEXITY

$$\text{err}_{\text{true}}(H) \leq \text{err}_{\text{train}}(H) + \tilde{O}\left(\sqrt{\frac{Td}{m}}\right)$$

T small	large	small
T large	→ 0	increase
	"BIAS"	"VARIANCE"

- **T** = number of rounds
- **d** = VC dimension of weak learner
- **m** = number of training examples

Bounding *true* error (a first guess)



THIS SOMETIMES DOES HAPPEN

MAY NEED TO STOP EARLY

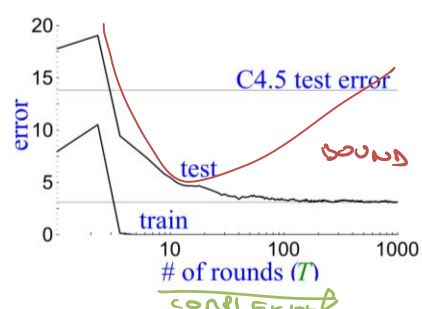
expect:

- training error to continue to drop (or reach zero)
- test error to increase when H_{final} becomes "too complex"

A typical run "contradicts" a naïve bound

NOT REALLY (SINCE ONLY AN UPPER BOUND)

BUT: NAIVE BOUND DOES NOT CAPTURE TRUE BEHAVIOR



(boosting C4.5 on "letter" dataset)

- test error does not increase, even after 1000 rounds
  - (total size > 2,000,000 nodes)
- test error continues to drop even after training error is zero!

Finer analysis: margins

[Schapire et al. 1998]

- key idea:
  - training error only measures whether classifications are right or wrong
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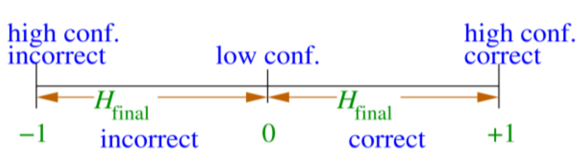
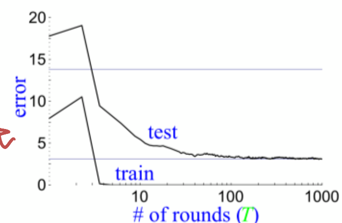
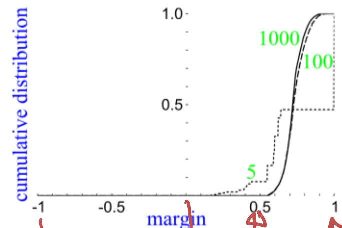


Empirical evidence: margin distribution

- margin distribution
  = cumulative distribution of margins of training examples



CRUDE MEASURE



INCORRECT TRAINING

HIGHLY CONFIDENT PRED

MODERATE CONFIDENCE

Empirical evidence: margin distribution

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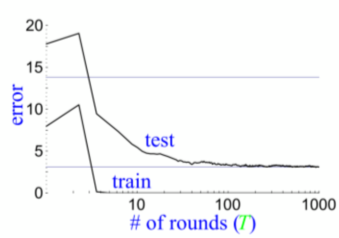

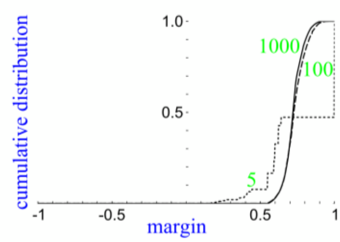

	# rounds		
	5	100	1000
train error	0.0	0.0	0.0
test error	8.4	3.3	3.1
% margins ≤ 0.5	7.7	0.0	0.0
minimum margin	0.14	0.52	0.55

Theoretical evidence: large margins ⇒ simple classifiers

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- Theorem: boosting tends to increase margins of training examples (given weak learning assumption)
- so:
  although final classifier is getting larger,
  margins are likely to be increasing,
  so final classifier actually getting close to a simpler classifier,
  driving down the test error

More technically…

Bound depends on:
- **d** = VC dim of weak learner
- **m** = #training examples
- **entire distribution of training margins**

New generalization bound:

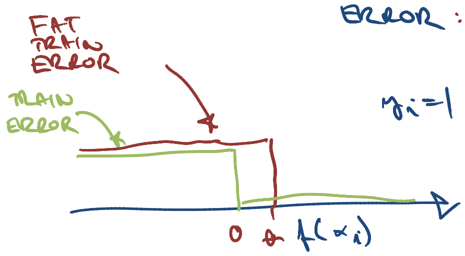
With high probability, for all $\theta > 0$

$$\mathrm{err}_{\mathrm{true}}(H) \leq \underbrace{\left(\frac{1}{m}\sum_{i=1}^{m}\delta\big(y_i f(x_i) < \theta\big)\right)} + \underbrace{\tilde{O}\left(\frac{\sqrt{d/m}}{\theta}\right)}$$

FAT TRAINING ERROR: INCREASES WITH θ

DROPS WITH θ

$y_i = 1$



More technically…

Previously

$$\mathrm{err}_{\mathrm{true}}(H) \leq \mathrm{err}_{\mathrm{train}}(H) + \tilde{O}\left(\sqrt{\frac{Td}{m}}\right)$$

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$\theta = 0$

USELESS FOR $\theta = 0$

BUT INDEP OF T!
(tighter if we can decrease fat error)

Practical advantages of AdaBoost

- fast
- simple and easy to program
- no parameters to tune (except T)

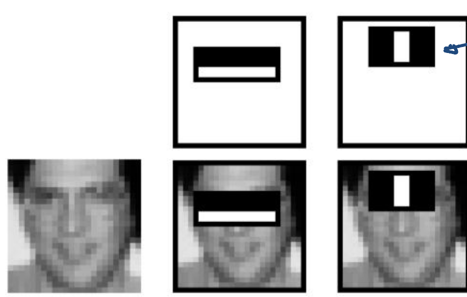
OVERFITTING REGIMES

- flexible — can combine with any learning algorithm
- no prior knowledge needed about weak learner
- provably effective, provided can consistently find rough rules of thumb
  - → shift in mind set — goal now is merely to find classifiers barely better than random guessing
- versatile
  - can use with data that is textual, numeric, discrete, etc.
  - has been extended to learning problems well beyond binary classification

Application: detecting faces

[Viola-Jones 2001]

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

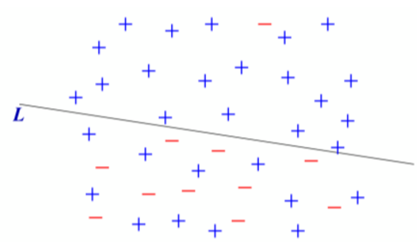


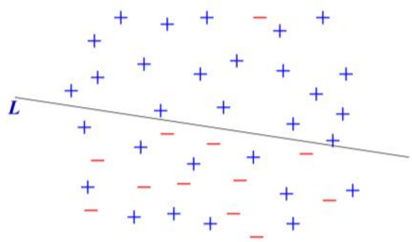
DEC. STUMPS OVER "DIFFERENCE" SUBIMAGES

- many clever tricks to make extremely fast and accurate

Caveats

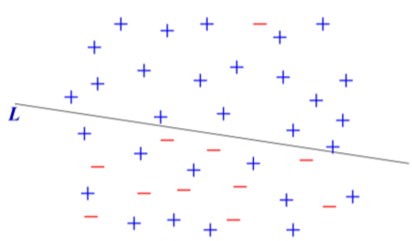
- performance of AdaBoost depends on data and weak learner
- consistent with theory, AdaBoost can fail if
  - weak classifiers too complex
    - $\longrightarrow$ overfitting
  - weak classifiers too weak ($\gamma_t \to 0$ too quickly)
    - $\longrightarrow$ underfitting
    - $\longrightarrow$ low margins $\longrightarrow$ overfitting
- empirically, AdaBoost seems especially susceptible to uniform noise





- ideally, want weak classifier that says:

$$h(x) = \begin{cases} +1 & \text{if } x \text{ above } L \\ \text{``don't know''} & \text{else} \end{cases}$$



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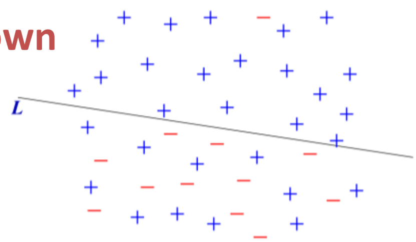
- problem: cannot express using "hard" predictions
- if must predict ± 1 below L, will introduce many "bad" predictions
  - need to "clean up" on later rounds
- dramatically increases time to convergence

"Hard" predictions can slow down learning!



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Confidence-rated Predictions

[Schapire-Singer 1999]

- useful to allow weak classifiers to assign confidences to predictions
- formally, allow $h_t : X \rightarrow \mathbb{R}$

$$\begin{aligned} \operatorname{sign}(h_t(x)) &= \text{prediction} \\ |h_t(x)| &= \text{"confidence"} \end{aligned}$$

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- use identical update:

BEFORE: $h_t(x_i) \in \{-1,1\}$

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \cdot \exp(-\alpha_t \, y_i \, h_t(x_i))$$

and identical rule for combining weak classifiers

Confidence-rated Predictions

[Schapire-Singer 1999]

- useful to allow weak classifiers to assign confidences to predictions
- formally, allow $h_t : X \to \mathbb{R}$

$$\begin{aligned} \mathrm{sign}(h_t(x)) &= \text{prediction} \\ |h_t(x)| &= \text{``confidence''} \end{aligned}$$

- use identical update:

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \cdot \exp(-\alpha_t \, y_i \, h_t(x_i))$$

and identical rule for combining weak classifiers
- question: how to choose α_t and h_t on each round

Confidence-rated Predictions

- saw earlier:

$$\text{training error}(H_{\text{final}}) \leq \prod_t Z_t = \frac{1}{m}\sum_i \exp\left(-y_i \sum_t \alpha_t h_t(x_i)\right)$$

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- therefore, on each round t, should choose $\alpha_t h_t$ to minimize:

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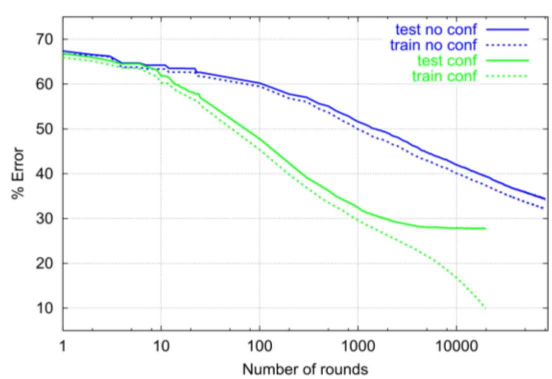
- in many cases (e.g., decision stumps), best confidence-rated weak classifier has simple form that can be found efficiently

Confidence-rated predictions help a lot!

- FASTER TO CONVERGE
- ALSO: FASTER TO OVERFIT IF DATA NOISY



% error	round first reached conf.	round first reached no conf.	speedup
40	268	16,938	63.2
35	598	65,292	109.2
30	1,888	>80,000	–

Loss in logistic regression

Logistic regression assumes:

& PROBABILISTIC INTERPRETATION

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

$f(x) = w_0 + \sum_j x_j w_j$

Loss in logistic regression

Logistic regression assumes:

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And tries to maximize conditional likelihood:

$$P(y_1, \ldots, y_m \,|\, x_1, \ldots, x_m, H) = \prod_{i=1}^{m} \frac{1}{1 + \exp(-y_i f(x_i))}$$

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Equivalent to minimizing log loss

$$\sum_{i=1}^{m} \ln\Big(1+\exp(-y_i f(x_i))\Big)$$

Loss in AdaBoost

Logistic regression equivalent to minimizing log loss

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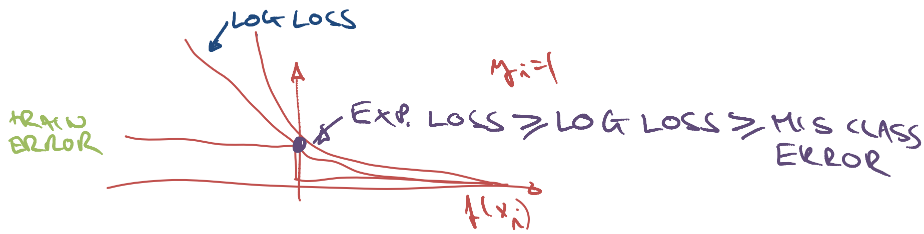
Loss in AdaBoost

Logistic regression equivalent to minimizing log loss

$$\sum_{i=1}^{m} \ln\Big(1+\exp(-y_i f(x_i))\Big)$$ LOG LOSS

Boosting minimizes similar loss function!

$$\frac{1}{m}\sum_{i=1}^{m} \exp(-y_i f(x_i)) = \prod_t Z_t$$



Logistic regression vs AdaBoost

Logistic regression:

- Minimize *log loss* (BINOMIAL)

$$\sum_{i=1}^{m} \ln\Big(1+\exp(-y_i f(x_i))\Big)$$

AdaBoost:

- Minimize *exponential loss*

$$\sum_{i=1}^{m} \exp(-y_i f(x_i))$$

Logistic regression vs AdaBoost

Logistic regression:

- Minimize *log loss*
  $$\sum_{i=1}^{m} \ln\left(1 + \exp(-y_i f(x_i))\right)$$
- Define
  $$f(x) = \sum_j w_j x_j$$
  where x_j's predefined

AdaBoost:

- Minimize *exponential loss*
  $$\sum_{i=1}^{m} \exp(-y_i f(x_i))$$
- Define
  $$f(x) = \sum_t \alpha_t h_t(x)$$
  where h_t's defined dynamically to fit the data

Logistic regression vs AdaBoost

Logistic regression:
LINEAR MODEL

- Minimize *log loss*
  $$\sum_{i=1}^{m} \ln\left(1 + \exp(-y_i f(x_i))\right)$$
- Define
  $$f(x) = \sum_j w_j x_j$$
  where x_j's predefined
- w_j's optimized jointly

AdaBoost:
LIN. MODEL IN A HUGE SPACE

- Minimize *exponential loss*
  $$\sum_{i=1}^{m} \exp(-y_i f(x_i))$$
- Define
  $$f(x) = \sum_t \alpha_t h_t(x)$$
  where h_t's defined dynamically to fit the data
- α_t's optimized one at a time

COORD. DESCENT

Benefits of model-fitting view

- immediate generalization to other loss functions
  - e.g. squared error for regression
  - e.g. logistic regression (by only changing one line of AdaBoost)

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Benefits of model-fitting view

- immediate generalization to other loss functions
  - e.g. squared error for regression
  - e.g. logistic regression (by only changing one line of AdaBoost)
- sensible approach for converting output of boosting into conditional probability estimates
- caveat: wrong to view AdaBoost as just an algorithm for minimizing exponential loss
  - other algorithms for minimizing same loss will (provably) give very poor performance
  - thus, this loss function cannot explain why AdaBoost "works"

What you should know about boosting

- **weak classifiers $\Rightarrow$ strong classifiers**
  - **weak:** slightly better than random on training data
  - **strong:** eventually zero error on training data
- AdaBoost prevents overfitting by increasing margins
- regimes when AdaBoost overfits
  - **weak learner too strong: use smaller trees** or **stop early**
  - **data noisy: stop early** or **regularize α_t**
- **AdaBoost** vs **Logistic Regression**
  - **exponential loss** vs **log loss**
  - **single-coordinate updates** vs **full optimization**