10701
Machine Learning

Ensemble methods and Boosting

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
- **Simple (a.k.a. weak) learners are bad**
  - High bias, can't solve hard learning problems

- Can we make all weak learners always good???
  - **No!!!**
  - **But often yes…**

Simplest approach: A "bucket of models"

- Input:
  - your top *T* favorite learners (or tunings)
    - $L_1,\ldots,L_T$
  - A dataset *D*
- Learning algorithm:
  - Use 10-CV to estimate the error of $L_1,\ldots,L_T$
  - Pick the best (lowest 10-CV error) learner L*
  - Train L* on *D* and return its hypothesis h*

Pros and cons of a "bucket of models"

- Pros:
  - Simple
  - Will give results not much worse than the best of the "**base learners**"
- Cons:
  - What if there's not a single best learner?
- Other approaches:
  - Vote the hypotheses (how would you weight them?)
  - Combine them some other way?
  - How about *learning* to combine the hypotheses?

Stacked learners: first attempt

- Input:
  - your top *T* favorite learners (or tunings)
    - $L_1,\ldots,L_T$
  - A dataset *D* containing (**x,**y), ….
- Learning algorithm:
  - Train $L_1,\ldots,L_T$ on *D* to get $h_1,\ldots,h_T$
  - Create a new dataset D’ containing (**x’,**y’),….
    - **x’** is a vector of the T predictions $h_1(\mathbf{x}),\ldots,h_T(\mathbf{x})$
    - y is the label y for **x**
  - Train new classifier on D’ to get h’ --- which combines the predictions!
- To predict on a new **x:**
  - Construct **x’** as before and predict h’(**x’**)

Pros and cons of stacking

- Pros:
  - Fairly simple
  - Slow, but easy to parallelize
- Cons:
  - What if there's not a single best *combination scheme*?
  - E.g.: for movie recommendation sometimes L1 is best for users with many ratings and L2 is best for users with few ratings.

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?

Comments

- Ensembles based on blending/stacking were key approaches used in successful applications (for example, the netflix competition)
  - Winning entries blended many types of classifiers
- Ensembles based on stacking are the main architecture used in Watson
  - Not all of the base classifiers/rankers are learned, however; some are hand-programmed.

Boosting [Schapire, 1989]

- Idea: given a weak learner, run it multiple times on (reweighted) training data, then let the 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:
  - A linear combination of the votes of the different classifiers weighted by their strength

- **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(i) – weight of *i* th training example ($\mathbf{x}^i$,y^i)
  - Interpretations:
    - *i* th training example counts as D(i) examples
    - If I were to "resample" data, I would get more samples of "heavier" data points

- **Now, in all calculations, whenever used, *i* th training example counts as D(i) "examples"**
  - e.g., MLE for Naïve Bayes, redefine *Count(Y=y)* to be weighted count

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t.
- Get weak classifier $h_t : X \to \mathbb{R}$.
- Choose $\alpha_t \in \mathbb{R}$.
- Update:

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

where Z_t is a normalization factor

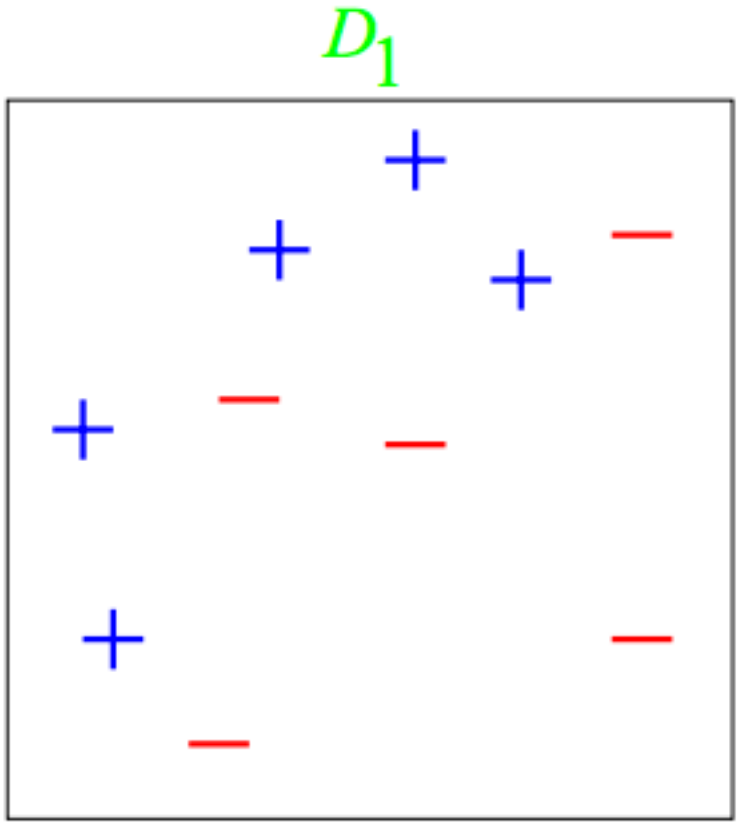
$$Z_t = \sum_{i=1}^{m} D_t(i) \exp(-\alpha_t y_i h_t(x_i))$$

Output the final classifier:

$$H(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right).$$

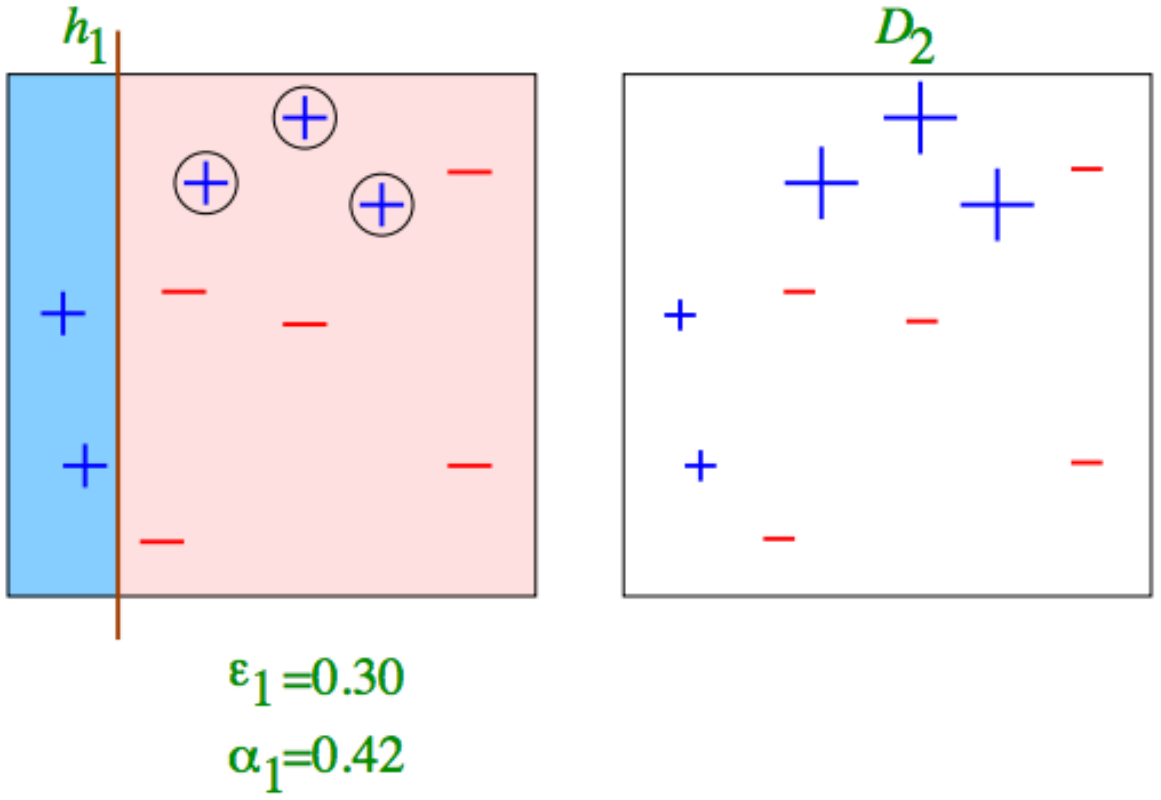
Figure 1: The boosting algorithm AdaBoost.

Boosting: A toy example



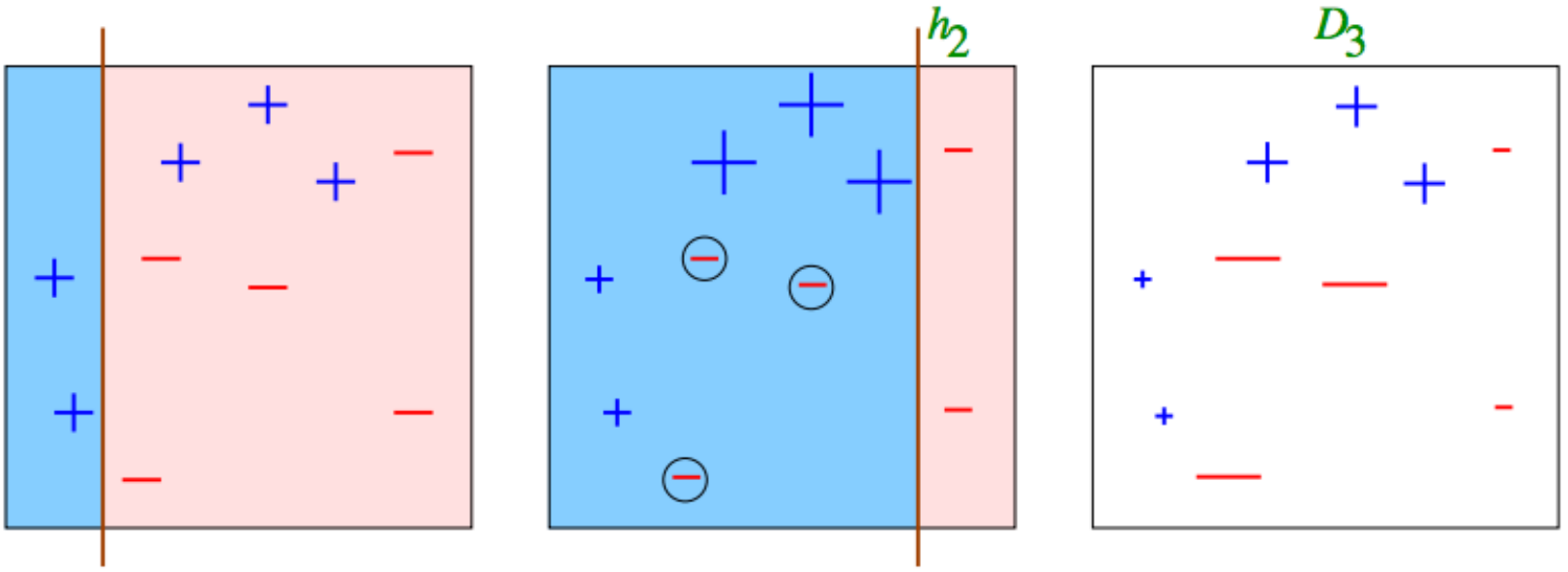
Boosting: A toy example

Round 1



Boosting: A toy example

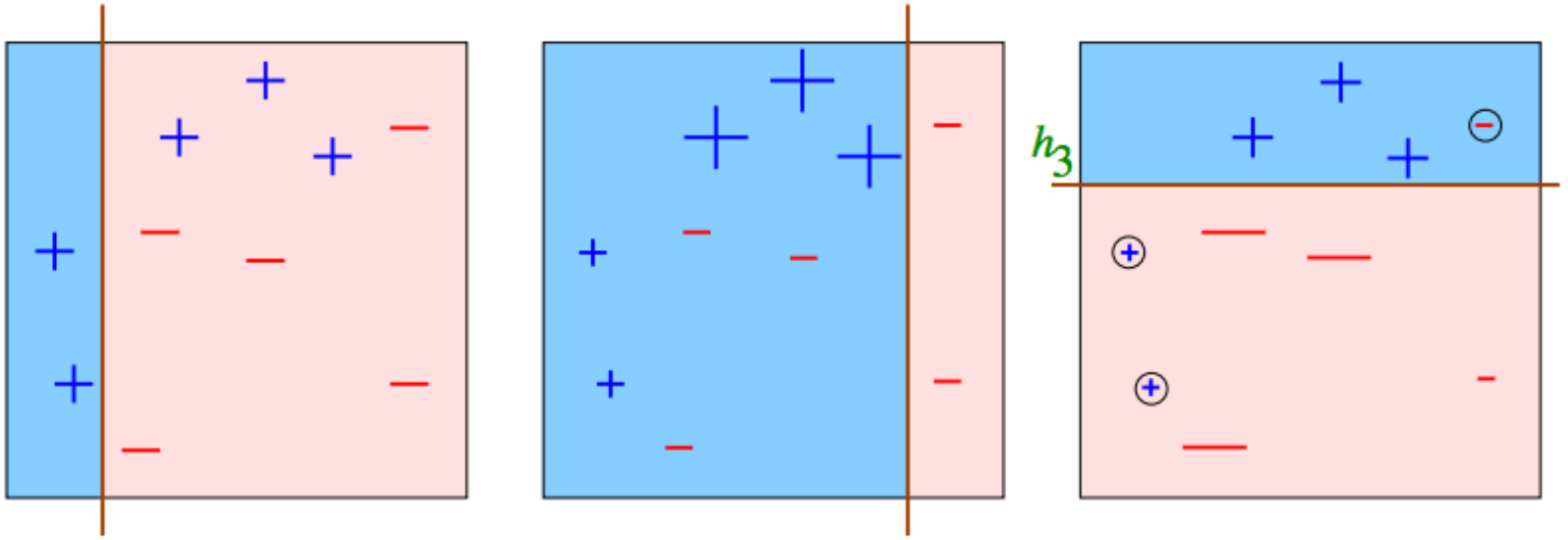
Round 2



Thanks, Rob Schapire

Boosting: A toy example

Round 3



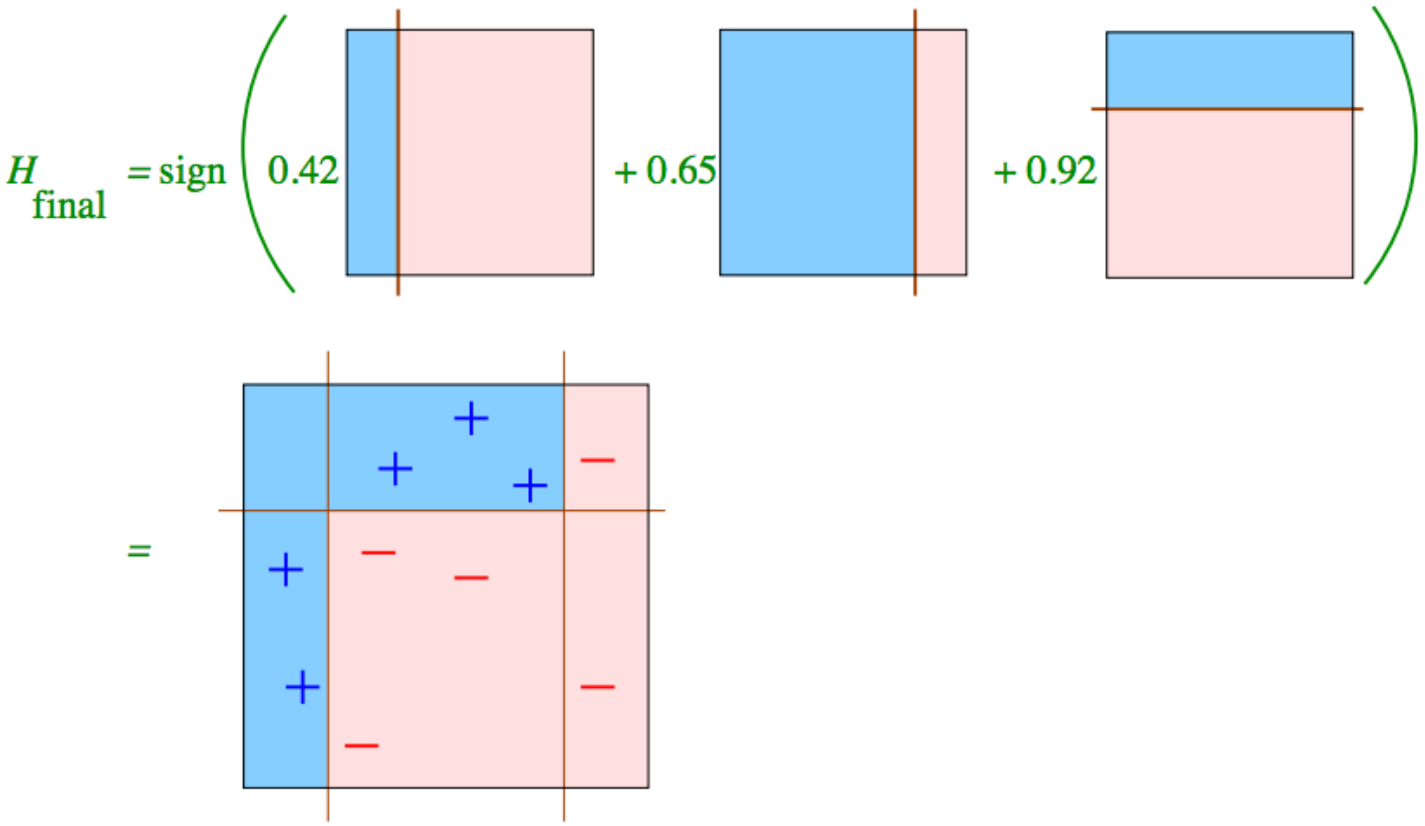
$\varepsilon_3 = 0.14$

$\alpha_3 = 0.92$

Thanks, Rob Schapire

Boosting: A toy example

Final Classifier



What α_t to choose for hypothesis h_t?

[Schapire, 1989]

Training error of final classifier is bounded by:

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

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

What α_t to choose for hypothesis h_t?

[Schapire, 1989]

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

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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

We can tighten this bound greedily, by choosing α_t and h_t on each iteration to minimize Z_t.

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

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[Schapire, 1989]

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

Define

$$\boxed{\epsilon_t = \sum_{i=1}^{m} D_t(i) \delta(h_t(x_i) \neq y_i)}$$

We can show that:

$$Z_t = (1-\varepsilon_t) \exp^{-\alpha_t} + \varepsilon_t \exp^{\alpha_t}$$

What α_t to choose for hypothesis h_t?

[Schapire, 1989]

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

$$Z_t = (1-\varepsilon_t)\exp^{-\alpha_t} + \varepsilon_t \exp^{\alpha_t}$$

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

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

Where:

$$\epsilon_t = \sum_{i=1}^{m} D_t(i)\delta(h_t(x_i) \neq y_i)$$

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

- Train base learner using distribution D_t.
- Get base classifier $h_t : X \to \mathbb{R}$.
- Choose $\alpha_t \in \mathbb{R}$.
- Update:

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

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

Strong, weak classifiers

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

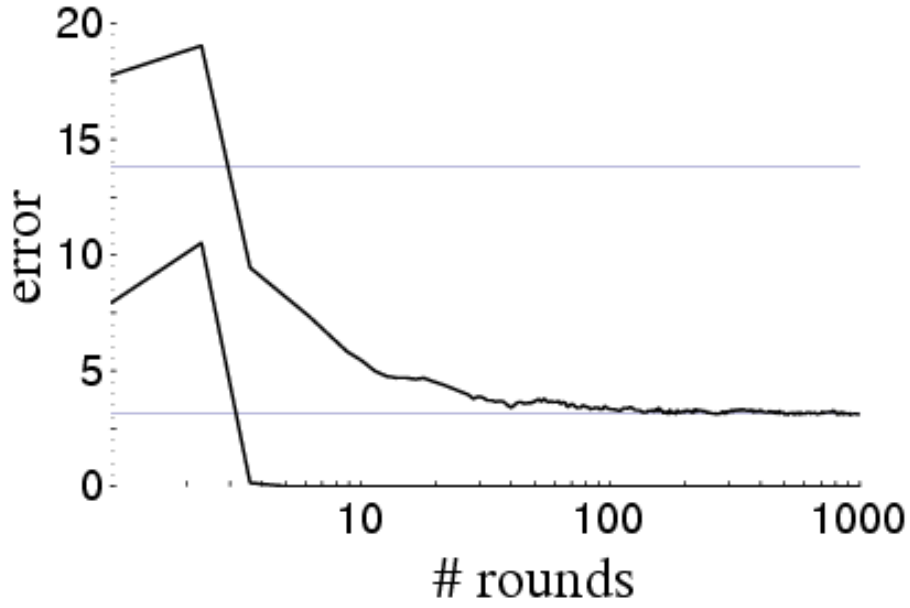
- If each classifier is (at least slightly) better than random
  - $\varepsilon_t < 0.5$

- With a few extra steps it can be shown that AdaBoost will achieve zero *training error* (exponentially fast):

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

Boosting results – Digit recognition

[Schapire, 1989]

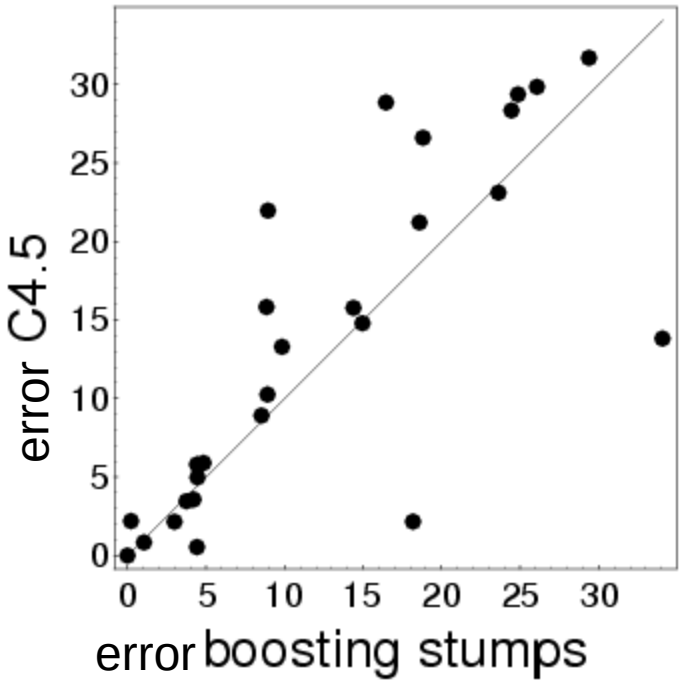


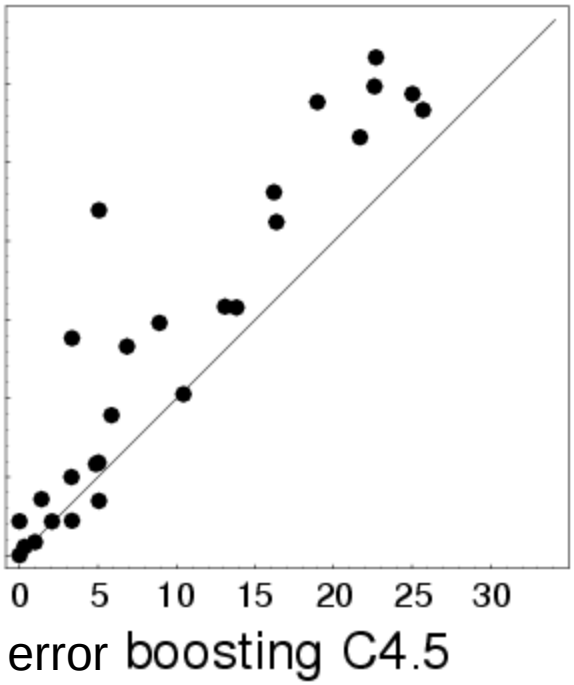
- Boosting often
  - Robust to overfitting
  - Test set error decreases even after training error is zero

Boosting: Experimental Results

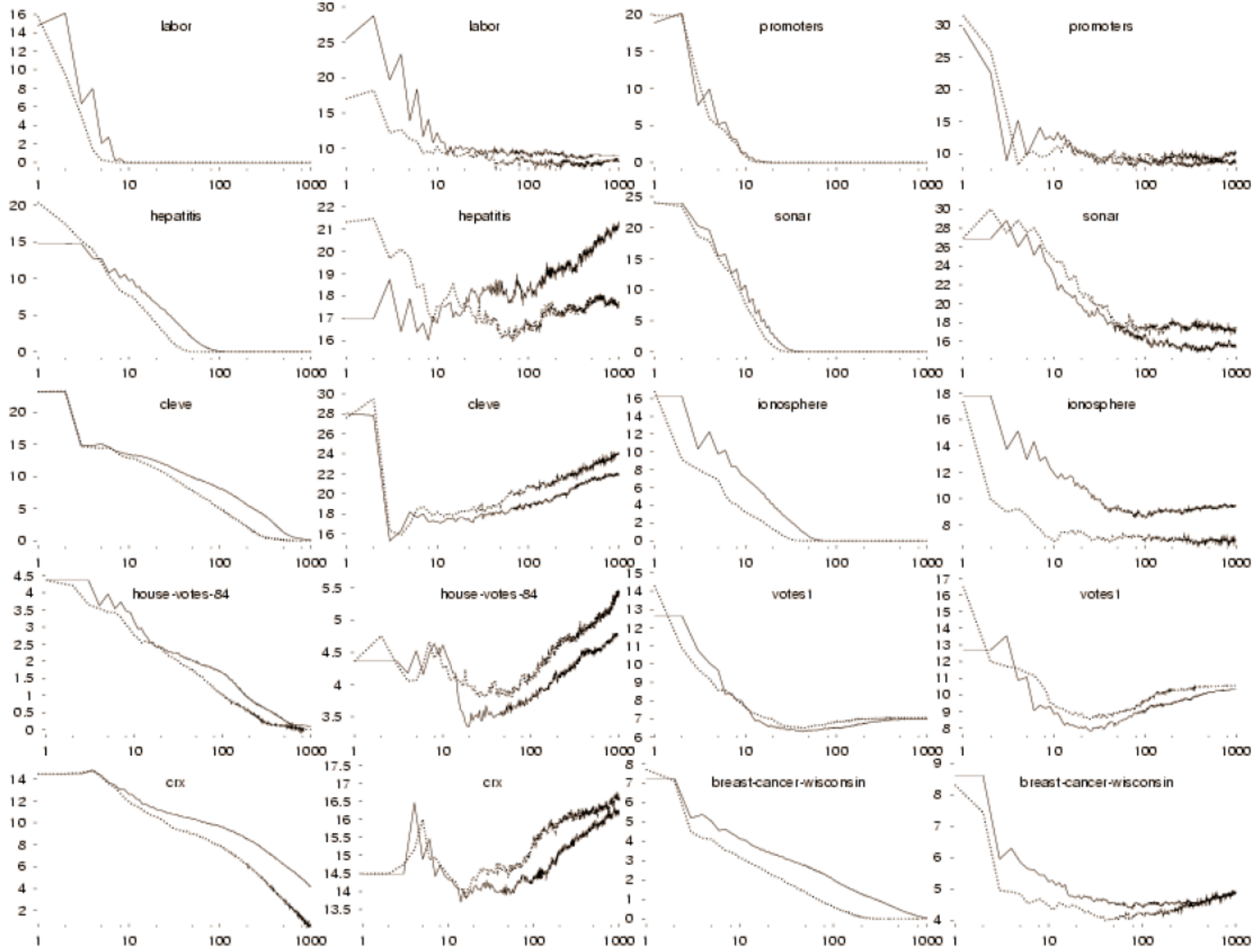
[Freund & Schapire, 1996]

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



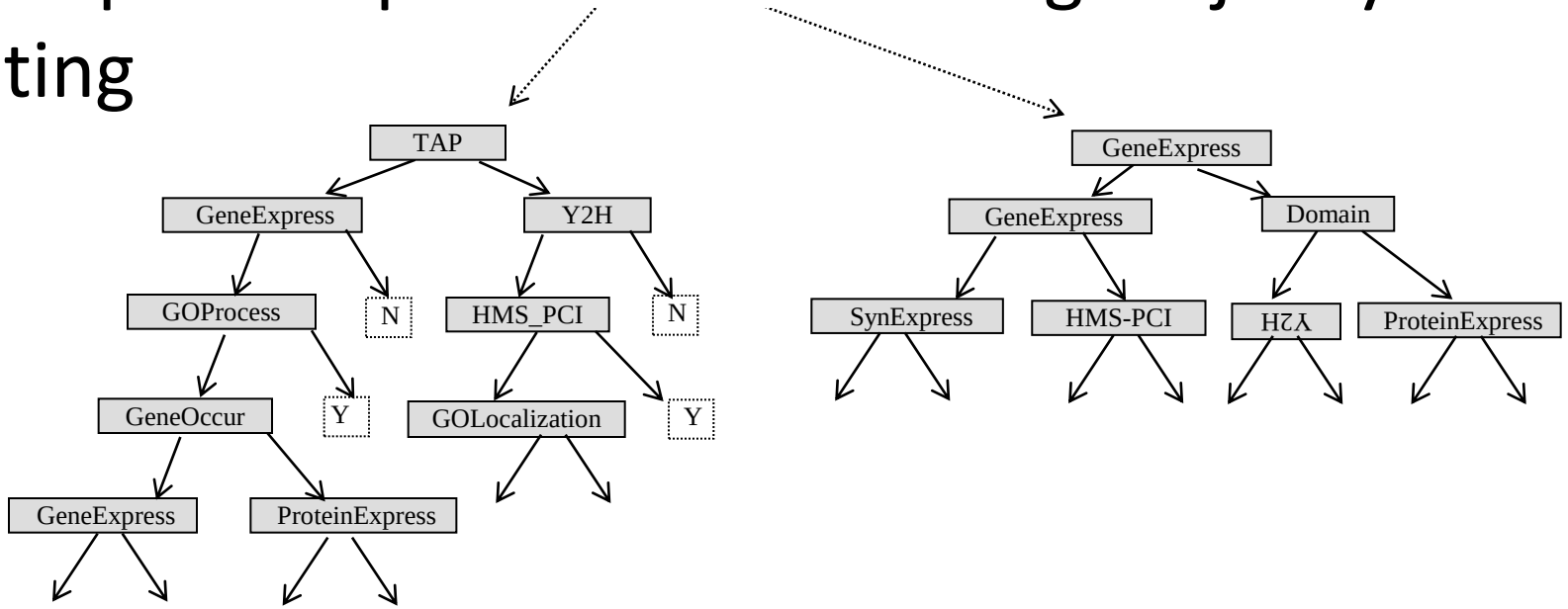


AdaBoost and AdaBoost.MH on Train (left) and Test (right) data from Irvine repository. [Schapire and Singer, ML 1999]



Random forest

- A collection of decision trees
- For each tree we select a subset of the attributes (recommended square root of |A|) and build tree using just these attributes
- An input sample is  sing majority voting



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
- Most popular application of Boosting:
  - Boosted decision stumps!
  - Very simple to implement, very effective classifier

Boosting and Logistic Regression

Logistic regression assumes:

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

And tries to maximize data likelihood:

$$P(\mathcal{D}|H) = \prod_{i=1}^{m} \frac{1}{1 + \exp(-y_i f(x_i))}$$

Equivalent to minimizing log loss

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

Boosting and Logistic Regression

Logistic regression equivalent to minimizing log loss

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

Boosting minimizes similar loss function!!

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

Both smooth approximations of 0/1 loss!

Logistic regression and Boosting

Logistic regression:

- Minimize loss fn

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

- Define

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

where x_j predefined

Boosting:

- Minimize loss fn

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

- Define

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

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

(not a linear classifier)

- Weights α_j learned incrementally