CSE546: Ensemble Learning - Bagging and Boosting
Winter 2012

Luke Zettlemoyer

Slides adapted from Carlos Guestrin, Nick Kushmerick, Padraig Cunningham

Voting (Ensemble Methods)

- Instead of learning a single classifier, learn **many weak classifiers** that are **good at different parts of the data**
- **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???**
  - force classifiers to learn about different parts of the input space? different subsets of the data?
  - weigh the votes of different classifiers?

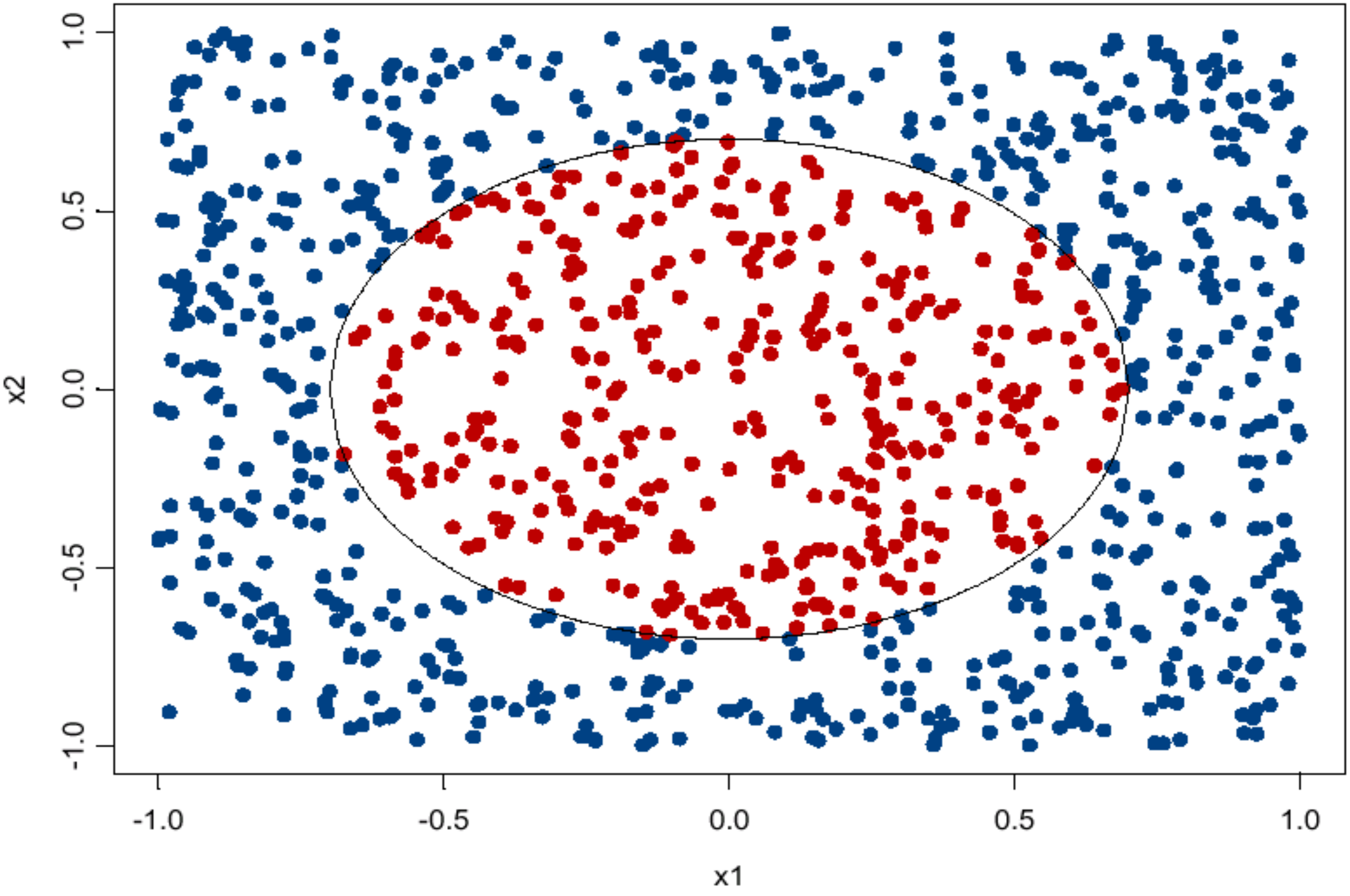
BAGGing = Bootstrap AGGregation

(Breiman, 1996)

- for i = 1, 2, …, K:
  - T_i ← randomly select M training instances with replacement
  - h_i ← learn(T_i) *[ID3, NB, kNN, neural net, …]*

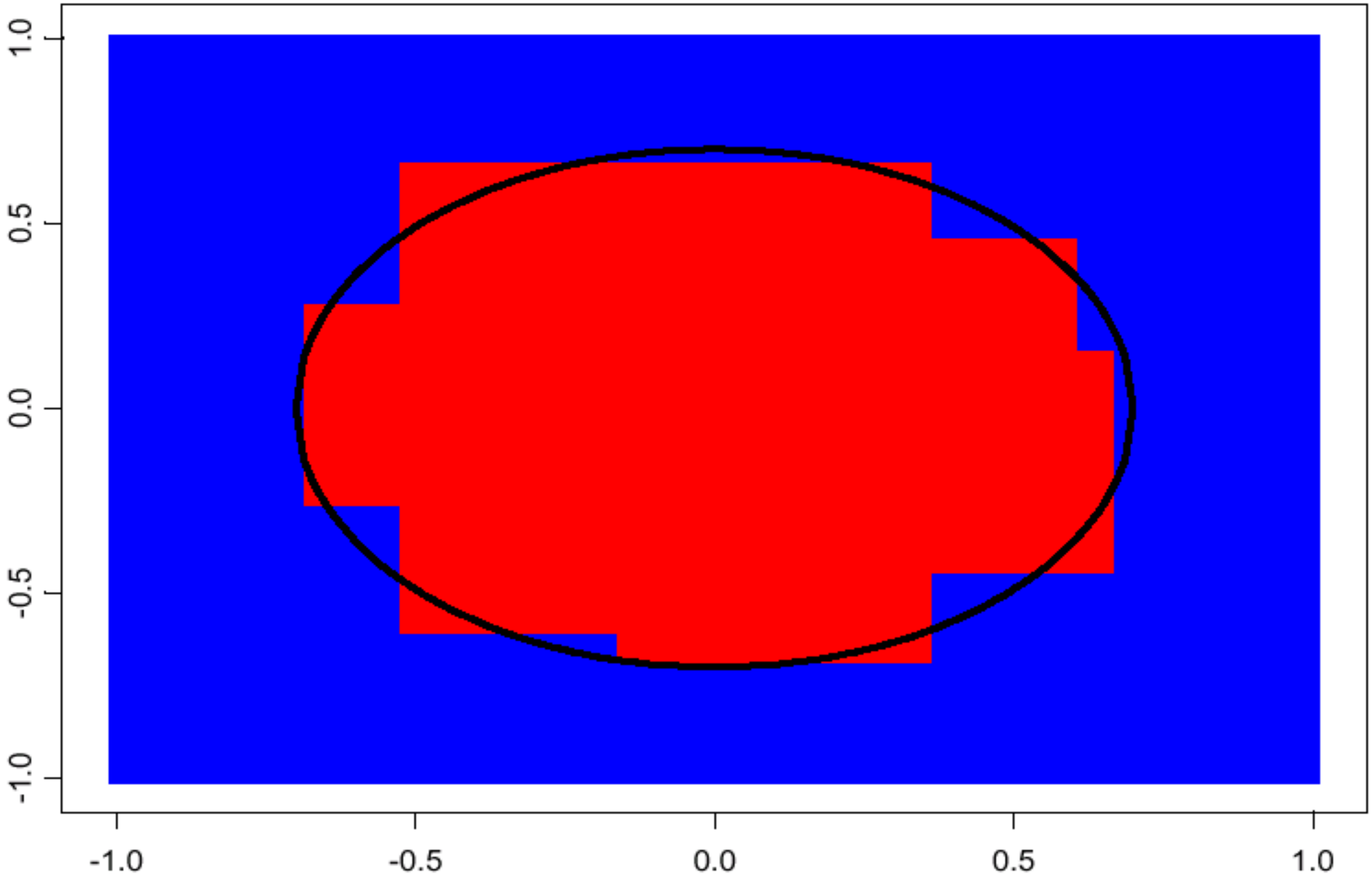
- Now combine the T_i together with uniform voting (w_i=1/K for all i)

Bagging Example

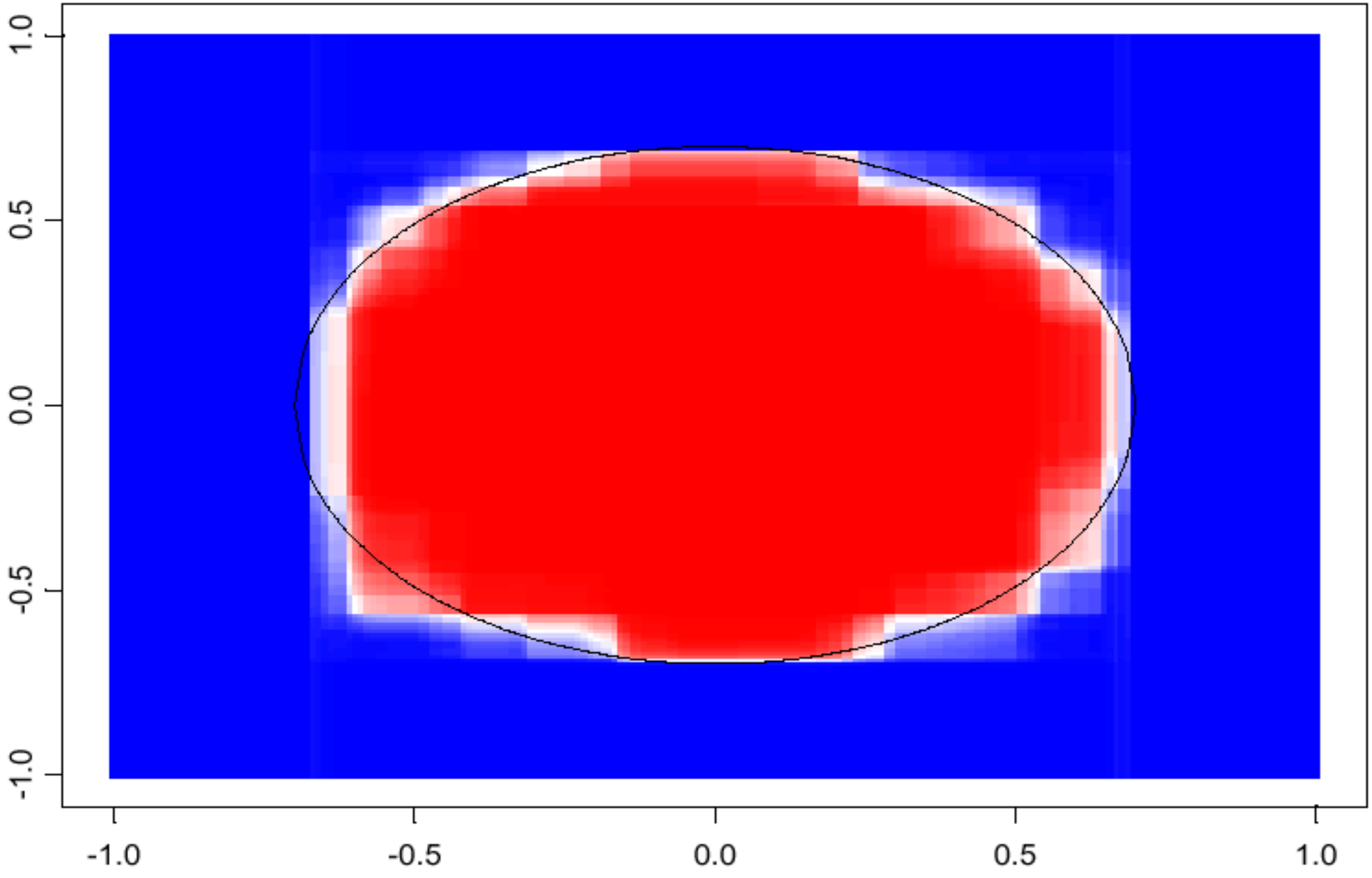


decision tree learning algorithm; very similar to ID3

CART decision boundary



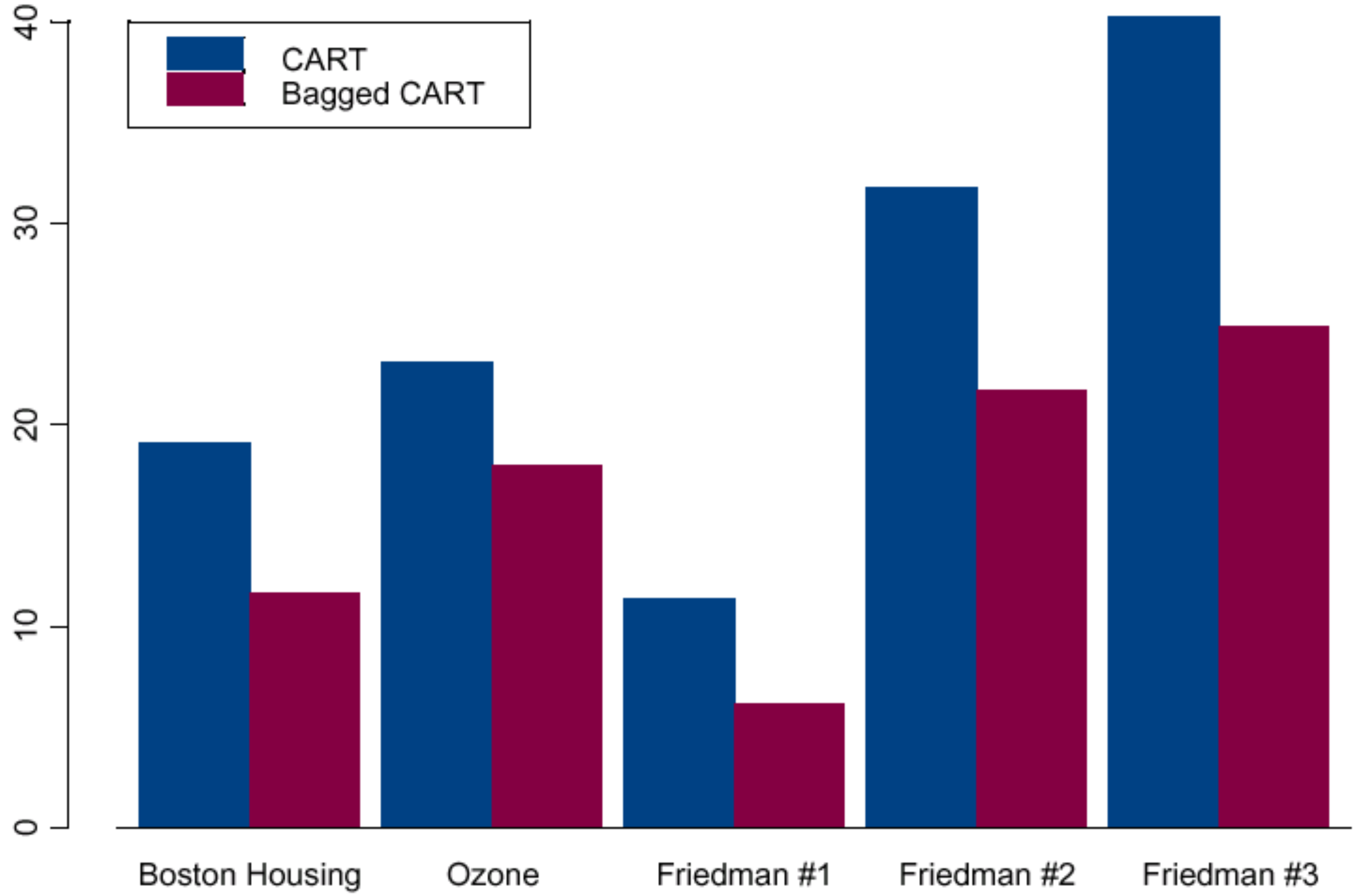
100 bagged trees



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

Regression results

Squared error loss



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 weak learners always good???
  - **No!!!**
  - **But often yes…**

Boosting [Schapire, 1989]

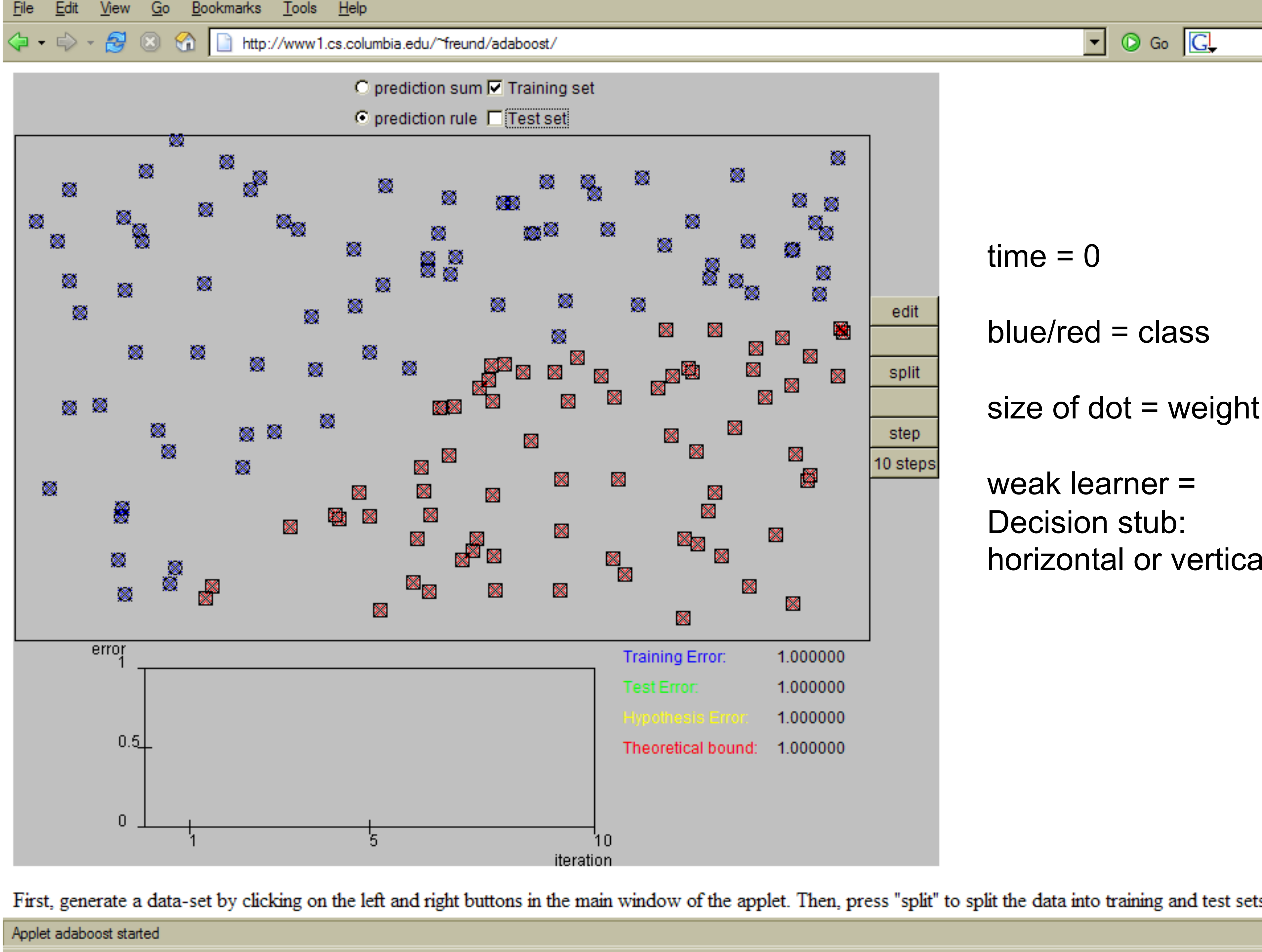
- Idea: given a weak learner, run it multiple times on (reweighted) training data, then let learned classifiers vote

- 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:

$$\boxed{h(x) = \text{sign}\left(\sum_i \alpha_i h_i(x)\right)}$$

- **Practically useful**
- **Theoretically interesting**



○ prediction sum ☑ Training set

● prediction rule □ Test set

Training Error: 1.000000

Test Error: 1.000000

Hypothesis Error: 1.000000

Theoretical bound: 1.000000

First, generate a data-set by clicking on the left and right buttons in the main window of the applet. Then, press "split" to split the data into training and test sets

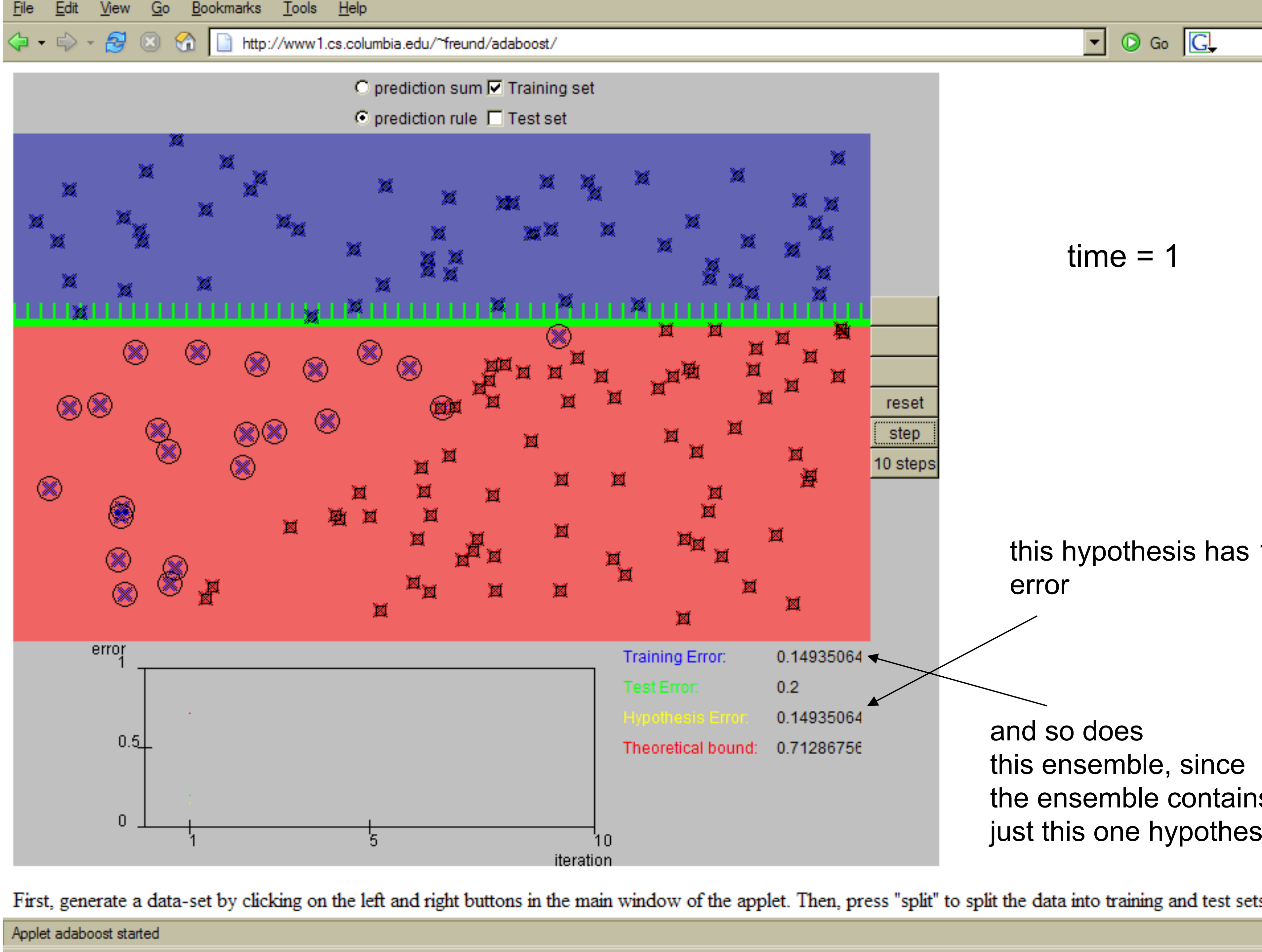
Applet adaboost started

time = 0

blue/red = class

size of dot = weight

weak learner = Decision stub: horizontal or vertica



http://www1.cs.columbia.edu/~freund/adaboost/

○ prediction sum ☑ Training set

● prediction rule □ Test set

Training Error:	0.14935064
Test Error:	0.2
Hypothesis Error:	0.14935064
Theoretical bound:	0.7128675

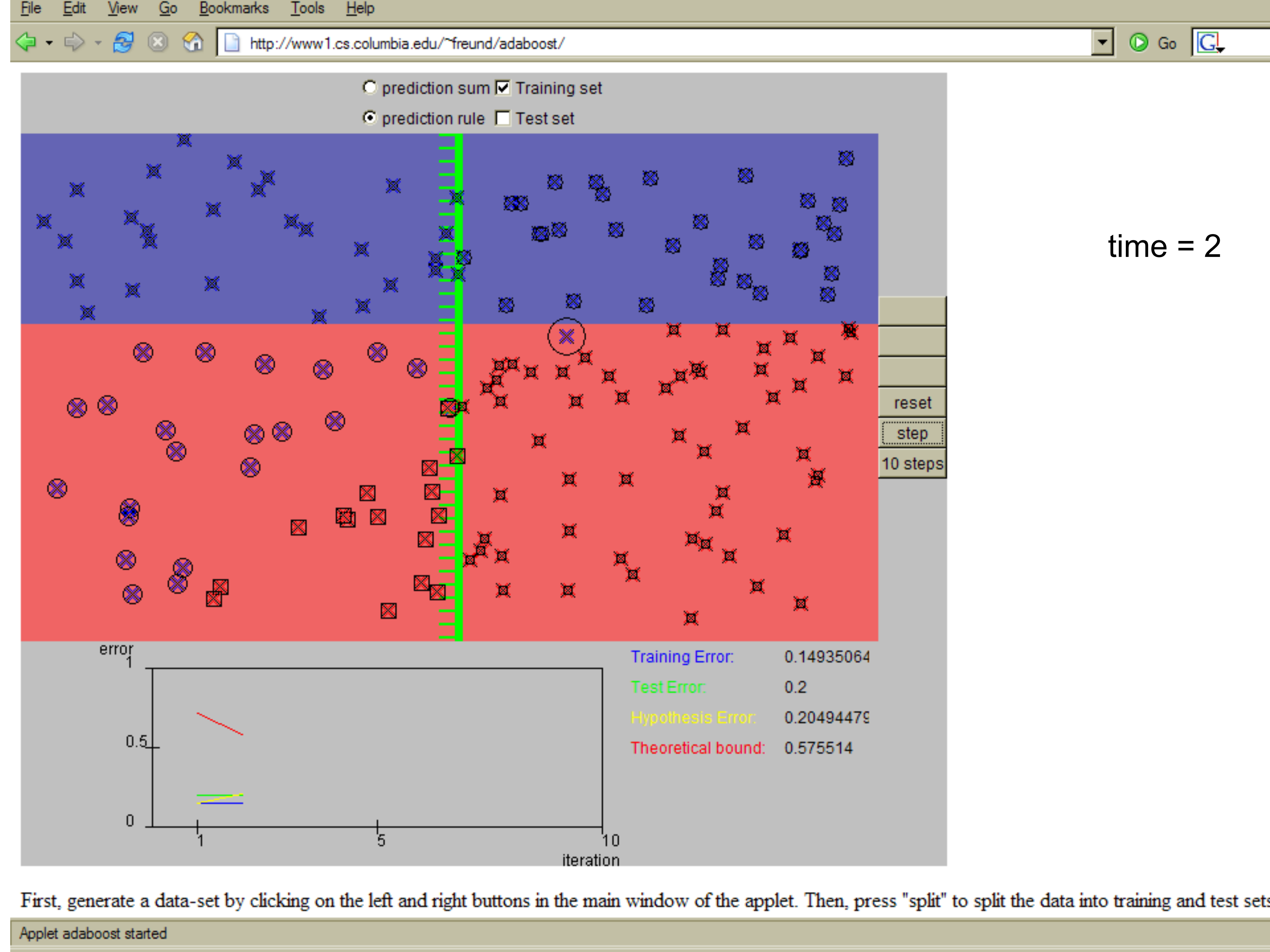
First, generate a data-set by clicking on the left and right buttons in the main window of the applet. Then, press "split" to split the data into training and test sets

time = 1

this hypothesis has
error

and so does
this ensemble, since
the ensemble contains
just this one hypothes

time = 2



http://www1.cs.columbia.edu/~freund/adaboost/

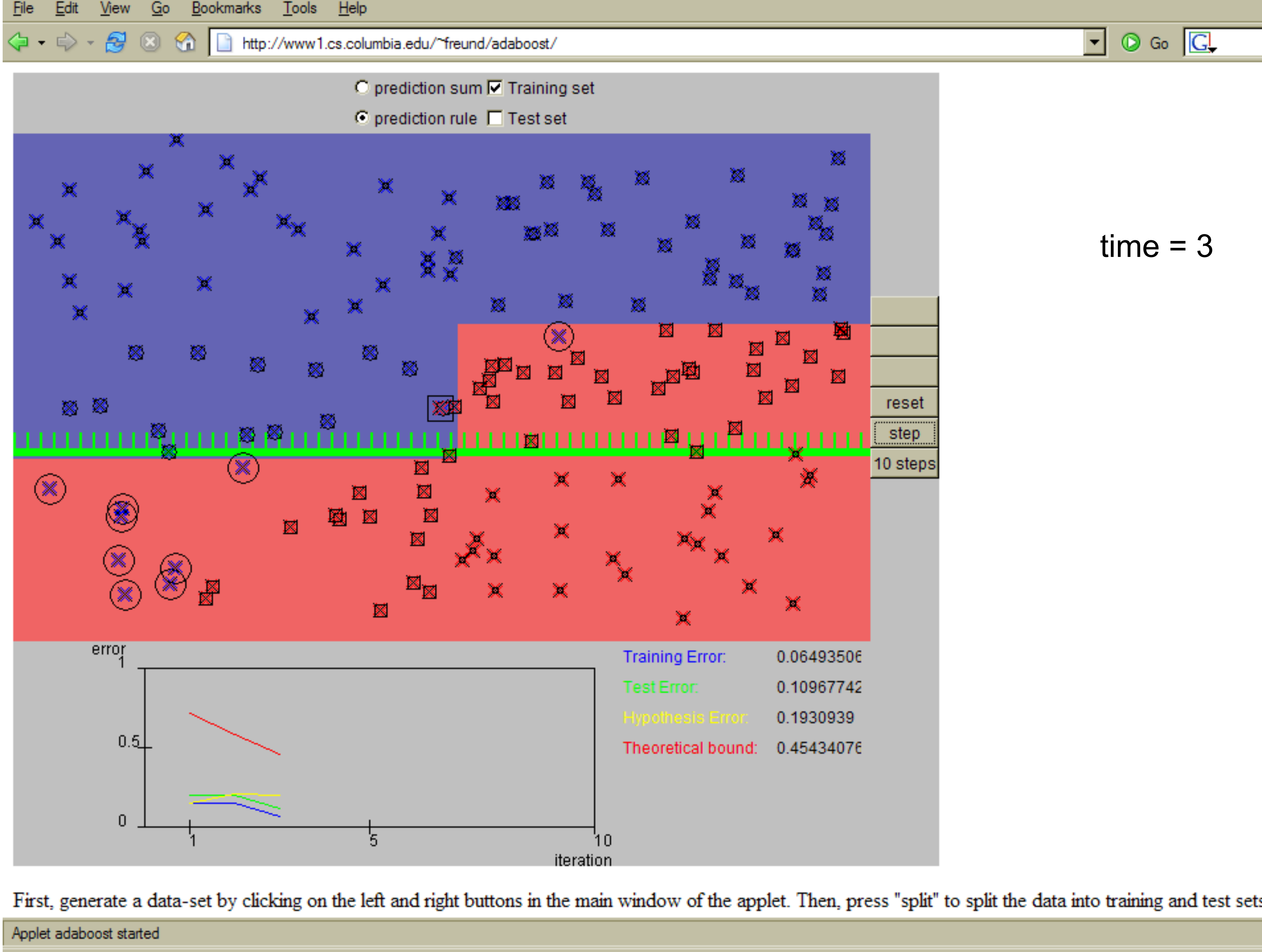
○ prediction sum ☑ Training set

● prediction rule □ Test set

Training Error:	0.14935064
Test Error:	0.2
Hypothesis Error:	0.20494479
Theoretical bound:	0.575514

First, generate a data-set by clicking on the left and right buttons in the main window of the applet. Then, press "split" to split the data into training and test sets

Applet adaboost started



http://www1.cs.columbia.edu/~freund/adaboost/

○ prediction sum ☑ Training set

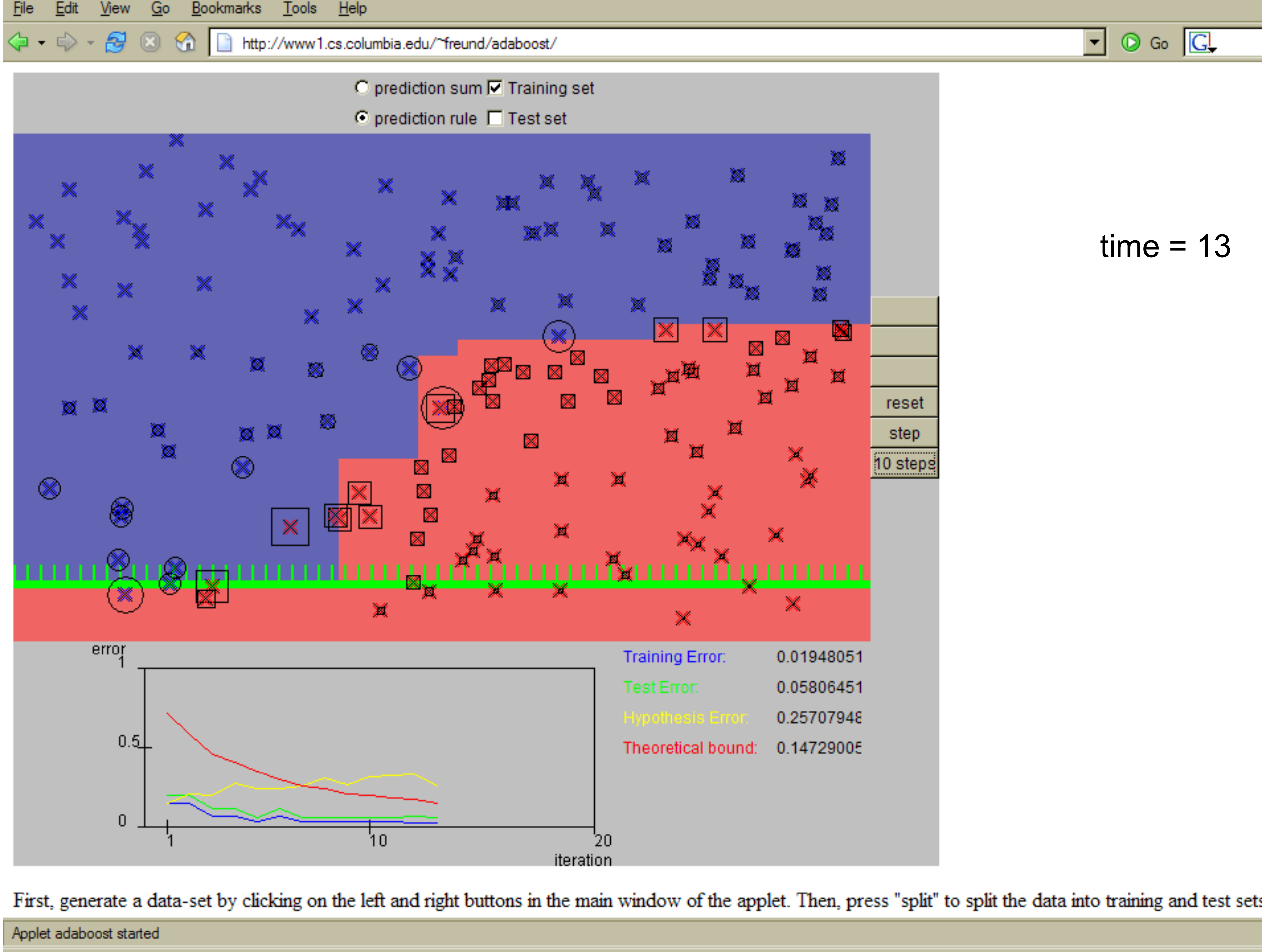
● prediction rule □ Test set

time = 3

Training Error:	0.06493506
Test Error:	0.10967742
Hypothesis Error:	0.1930939
Theoretical bound:	0.45434076

First, generate a data-set by clicking on the left and right buttons in the main window of the applet. Then, press "split" to split the data into training and test sets

Applet adaboost started



http://www1.cs.columbia.edu/~freund/adaboost/

○ prediction sum ☑ Training set

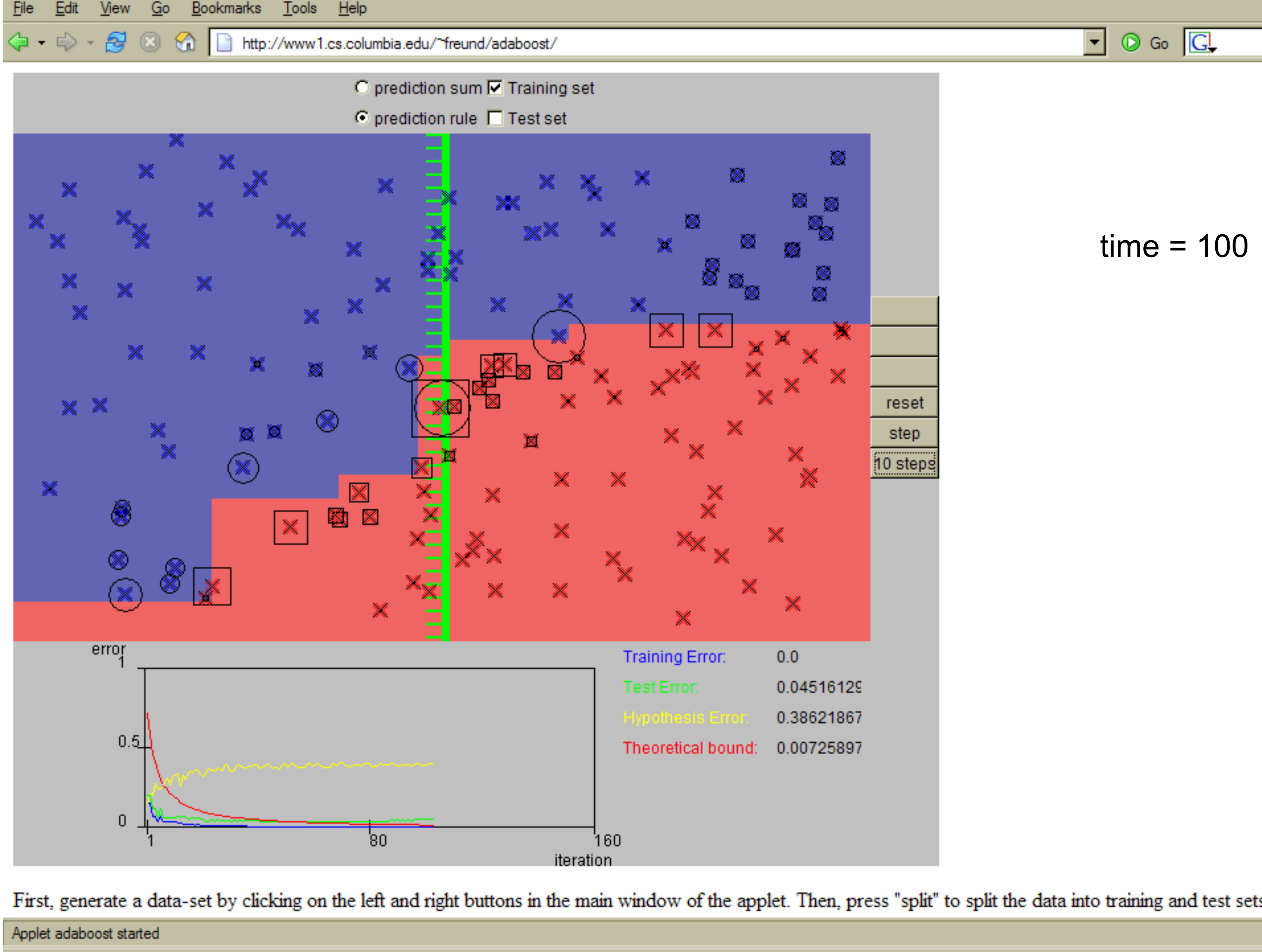
● prediction rule □ Test set

```
Training Error:       0.01948051
Test Error:           0.05806451
Hypothesis Error:     0.25707948
Theoretical bound:    0.14729005
```

First, generate a data-set by clicking on the left and right buttons in the main window of the applet. Then, press "split" to split the data into training and test sets

Applet adaboost started

time = 13



http://www1.cs.columbia.edu/~freund/adaboost/

○ prediction sum ☑ Training set

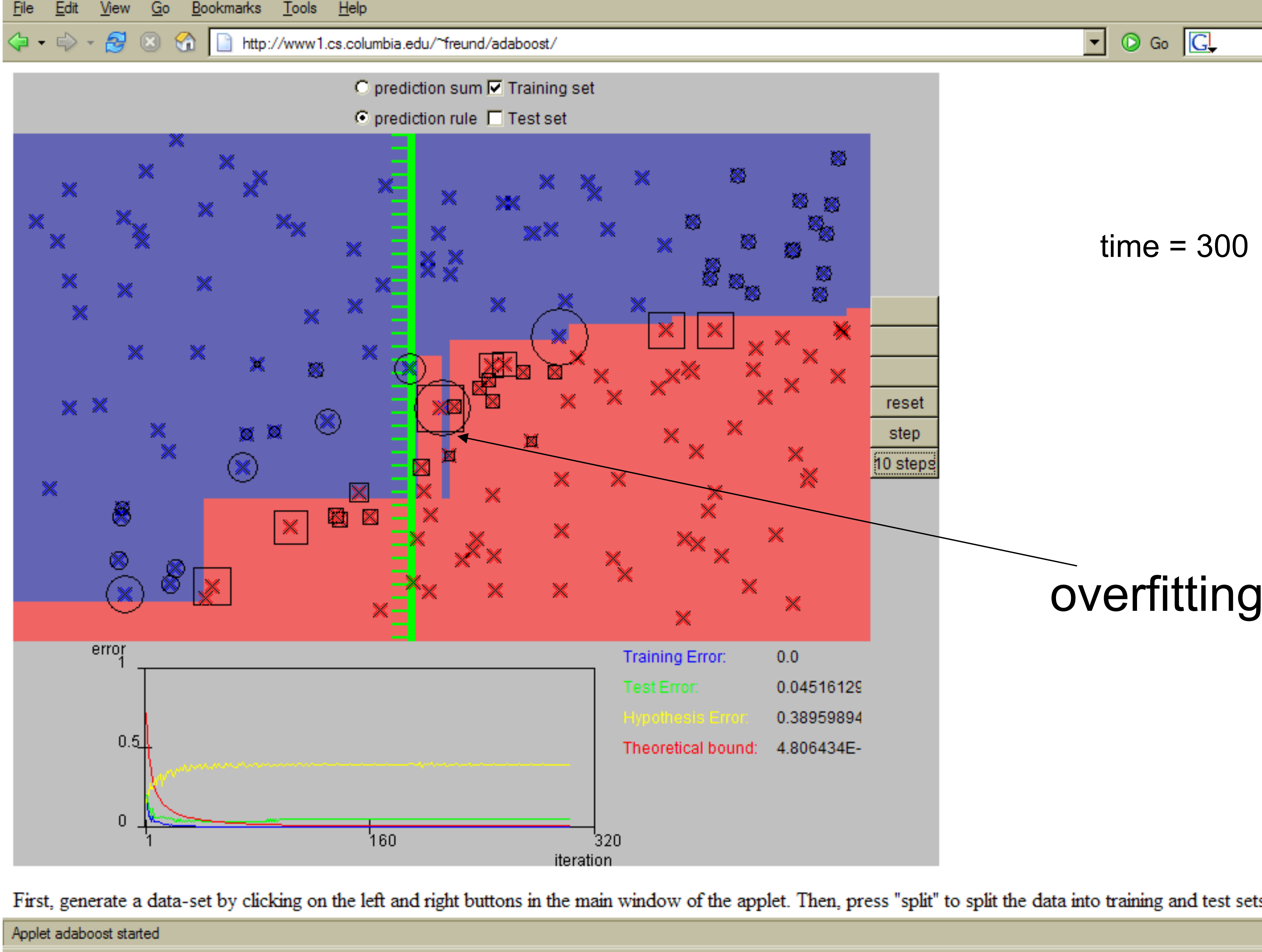
● prediction rule □ Test set

Training Error:	0.0
Test Error:	0.04516129
Hypothesis Error:	0.38621867
Theoretical bound:	0.00725897

time = 100

First, generate a data-set by clicking on the left and right buttons in the main window of the applet. Then, press "split" to split the data into training and test sets

Applet adaboost started



http://www1.cs.columbia.edu/~freund/adaboost/

○ prediction sum ☑ Training set

● prediction rule □ Test set

Training Error: 0.0

Test Error: 0.04516129

Hypothesis Error: 0.38959894

Theoretical bound: 4.806434E-

First, generate a data-set by clicking on the left and right buttons in the main window of the applet. Then, press "split" to split the data into training and test sets

Applet adaboost started

time = 300

overfitting

Learning from weighted data

- **Consider a weighted dataset**
  - D(i) – weight of *i* th training example ($\mathbf{x}^i$,y^i)
  - Interpretations:
    - *i* th training example counts as if it occurred D(i) times
    - If I were to "resample" data, I would get more samples of "heavier" data points
- **Now, always do weighted calculations:**
  - e.g., MLE for Naïve Bayes, redefine *Count(Y=y)* to be weighted count:

$$Count(Y = y) = \sum_{j=1}^{n} D(j)\delta(Y^j = y)$$

  - setting D(j)=1 (or any constant value!), for all j, will recreates unweighted case

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:

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

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.

How? Many possibilities. Will see one shortly!

Why? Reweight the data: examples *i* that are misclassified will have higher weights!

- $y_i h_t(x_i) > 0$ → h_i correct
- $y_i h_t(x_i) < 0$ → h_i wrong
- h_i correct, $\alpha_t > 0$ → $D_{t+1}(i) < D_t(i)$
- h_i wrong, $\alpha_t > 0$ → $D_{t+1}(i) > D_t(i)$

Final Result: linear sum of “base” or “weak” classifier outputs.

$$\epsilon_t = P_{i\sim D_t(i)}[h_t(\mathbf{x}^i) \neq y^i]$$

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

Given: $(x_1, y_1), \ldots, (x_m, y_m)$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

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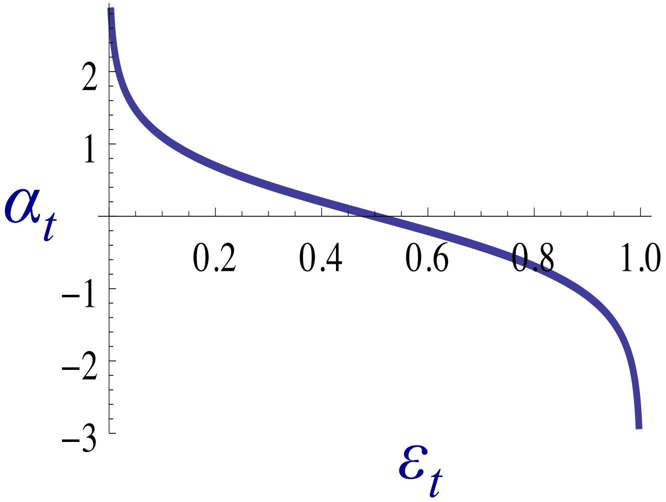
- Update:

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

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

- ε_t : error of h_t, weighted by D_t
  - $0 \leq \varepsilon_t \leq 1$
- α_t :
  - No errors: ε_t=0 → α_t=∞
  - All errors: ε_t=1 → α_t=−∞
  - Random: ε_t=0.5 → α_t=0



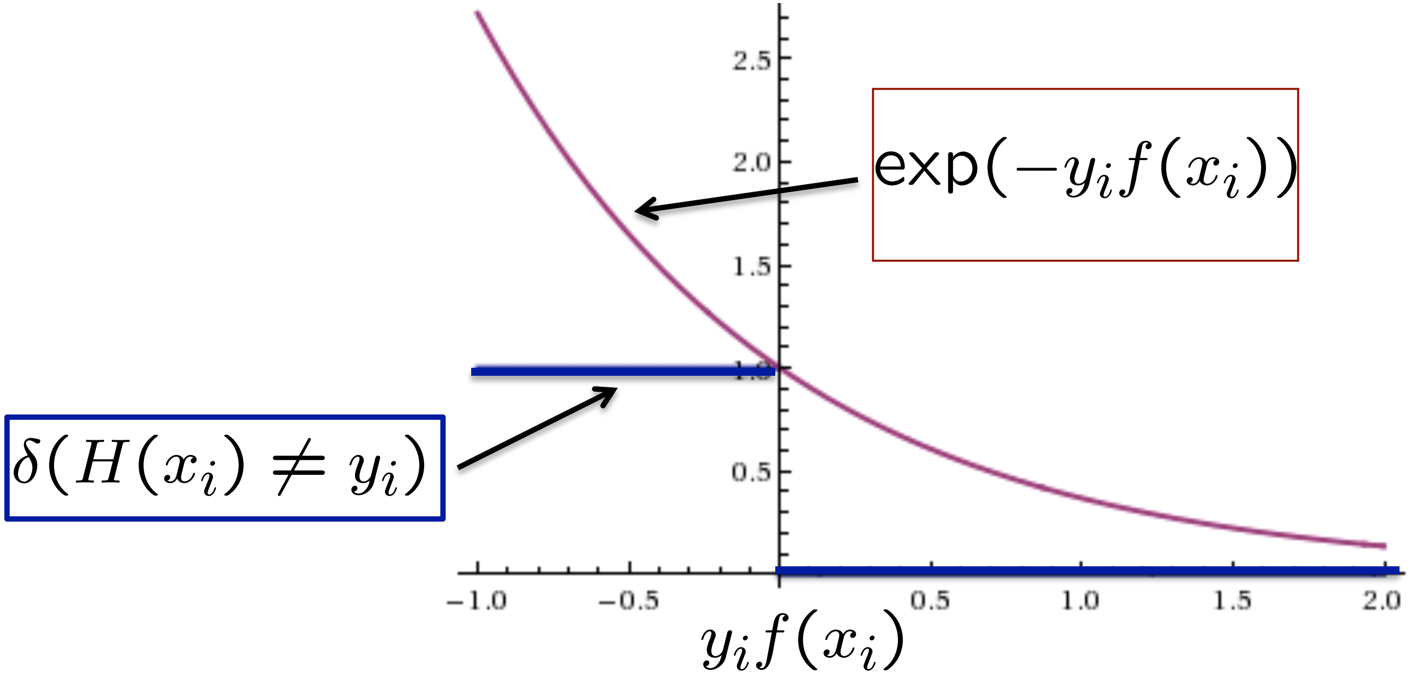
What α_t to choose for hypothesis h_t?

[Schapire, 1989]

Idea: choose α_t to minimize a bound on training error!

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

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



What α_t to choose for hypothesis h_t?

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Idea: choose α_t to minimize a bound on training error!

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

Where

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

And

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

This equality isn't obvious! Can be shown with algebra (telescoping sums)!

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 $Z_{t.}$
- h_t is estimated as a black box, but can we solve for α_t?

Summary: choose α_t to minimize *error bound*

[Schapire, 1989]

We can squeeze this bound by choosing α_t on each iteration to minimize $Z_{t.}$

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

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

For boolean Y: differentiate, set equal to 0, there is a closed form solution! [Freund & Schapire ’97]:

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

Strong, weak classifiers

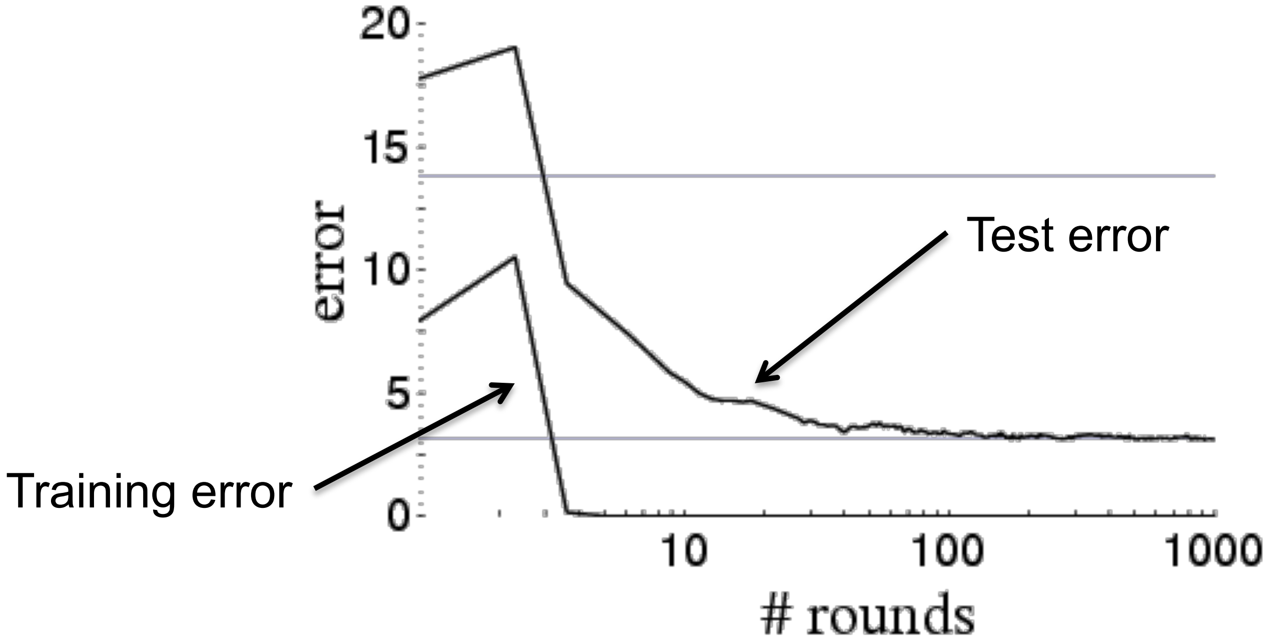
- If each classifier is (at least slightly) better than random: $\varepsilon_t < 0.5$
- Another bound on error:

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

- What does this imply about the training error?
  - Will reach zero!
  - Will get there exponentially fast!
- Is it hard to achieve better than random training error?

Boosting results – Digit recognition

[Schapire, 1989]



- Boosting:
  - Seems to be robust to overfitting
  - Test error can decrease even after training error is zero!!!

Boosting generalization error bound

[Freund & Schapire, 1996]

$$error_{true}(H) \quad \leq \quad error_{train}(H) + \tilde{\mathcal{O}}\left(\sqrt{\frac{Td}{m}}\right)$$

Constants:

- *T*: number of boosting rounds
  - Higher T → Looser bound, *what does this imply?*
- *d*: VC dimension of weak learner, measures complexity of classifier
  - Higher d → bigger hypothesis space → looser bound
- *m*: number of training examples
  - more data → tighter bound

Boosting generalization error bound

[Freund & Schapire, 1996]

$$error_{true}(H) \quad \leq \quad error_{train}(H) + \tilde{\mathcal{O}}\left(\sqrt{\frac{Td}{m}}\right)$$

Constants:

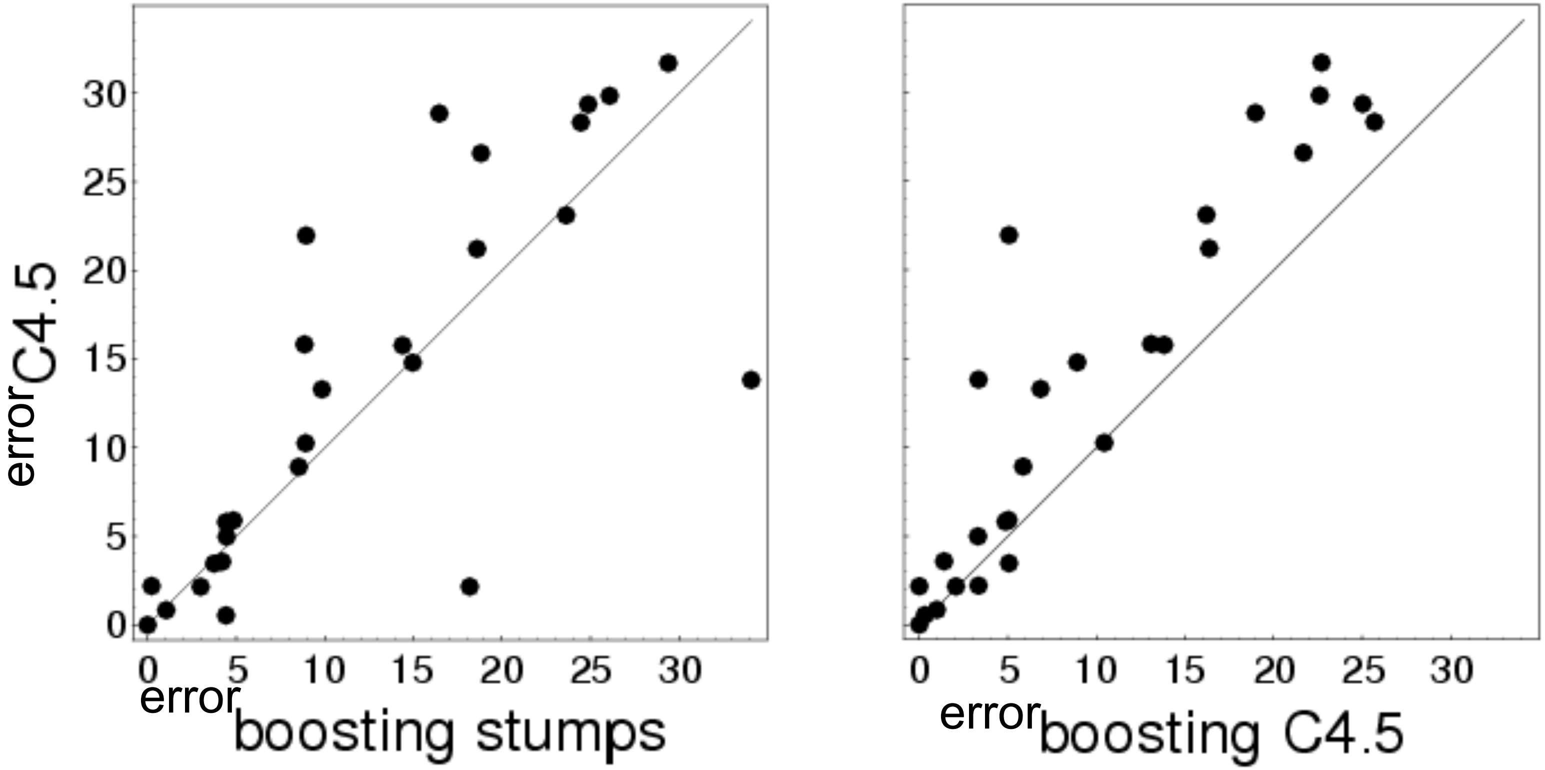
- **Theory does not match practice**:
  - Robust to overfitting
  - Test set error decreases even after training error is zero
- **Need better analysis tools**
  - we'll come back to this later in the quarter

– more data → tighter bound

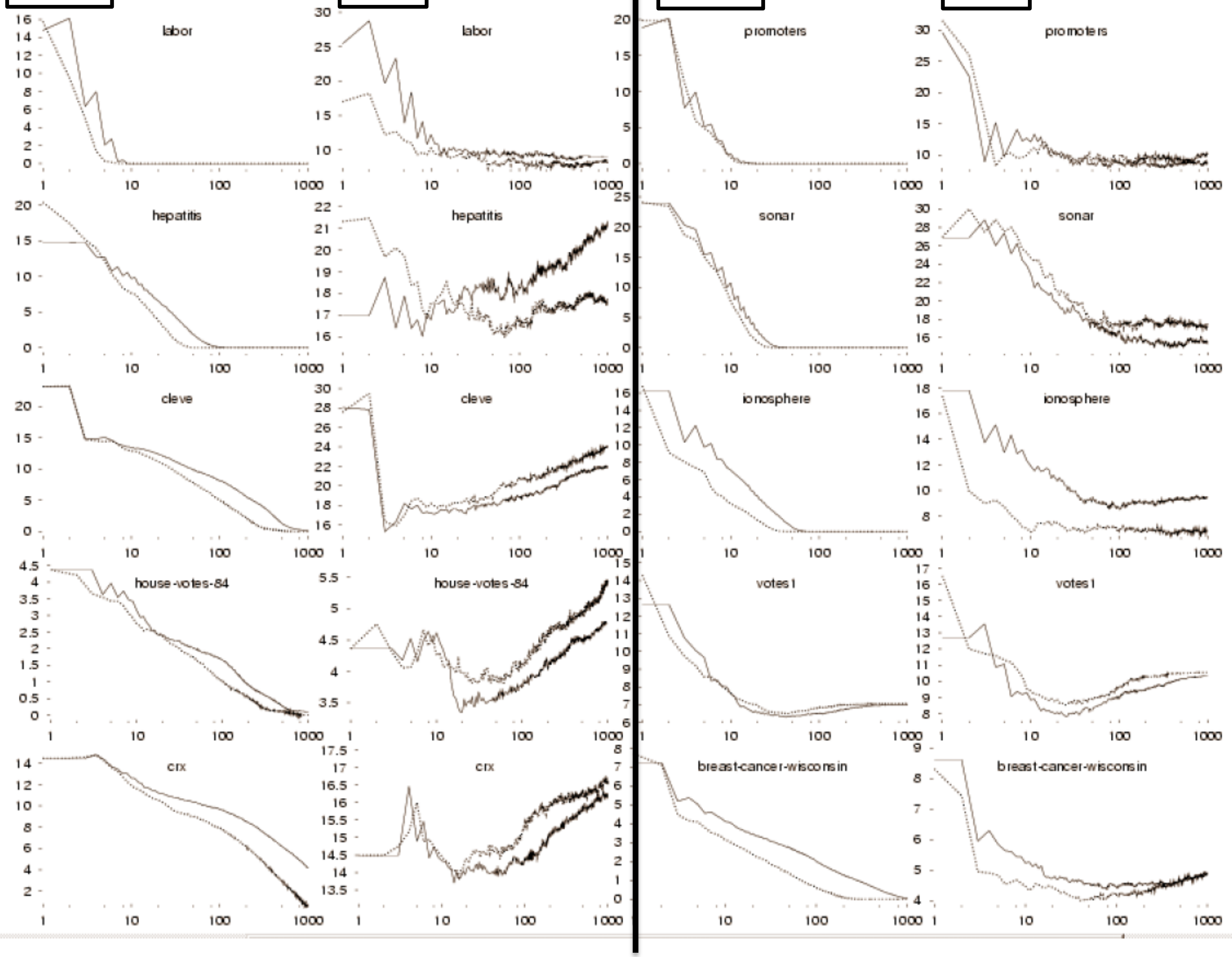
Boosting: Experimental Results

[Freund & Schapire, 1996]

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



A[illegible]nd AdaBoost.MH on [illegible]ft) and Test (right) dat[illegible]ne repository. [S[illegible]nd Singer, ML 1999]



Logistic Regression as Minimizing Loss

Logistic regression assumes:

$$P(Y=1|X) = \frac{1}{1+\exp(f(x))} \qquad f(x) = w_0 + \sum_i w_i h_i(x)$$

And tries to maximize data likelihood, for Y={-1,+1}:

$$P(y_i|\mathbf{x}_i) = \frac{1}{1+e^{-y_i f(\mathbf{x}_i)}} \qquad \ln P(\mathcal{D}_Y \mid \mathcal{D}_{\mathbf{X}}, \mathbf{w}) = \sum_{j=1}^{N} \ln P(y^j \mid \mathbf{x}^j, \mathbf{w})$$

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

Equivalent to minimizing *log loss*:

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

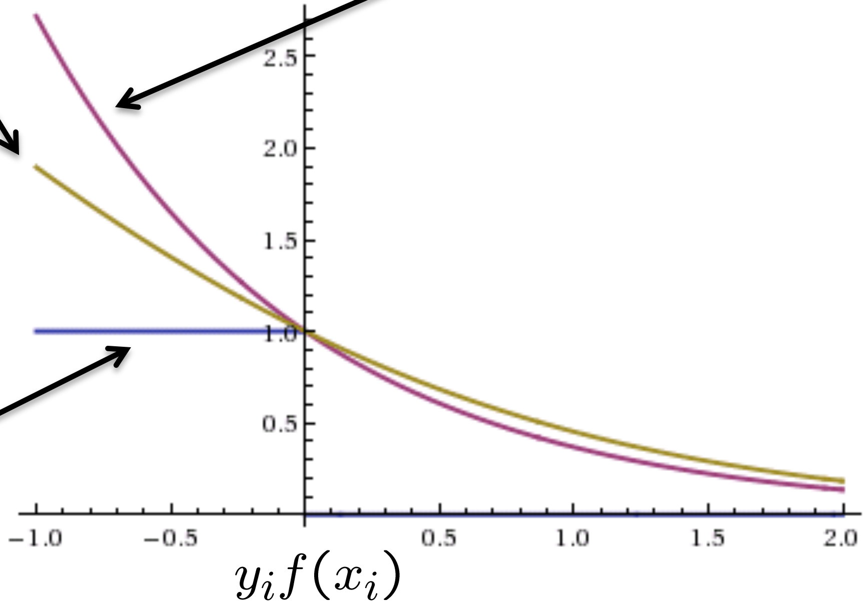
Boosting and Logistic Regression

Logistic regression equivalent to minimizing log loss:

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

Boosting minimizes similar loss function:

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



$$\delta(H(x_i) \neq y_i)$$

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

- Jointly optimize parameters $w_0, w_1, \ldots w_n$ via gradient ascent.

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

- Weights α_j learned incrementally (new one for each training pass)

What you need to know about Boosting

- Combine weak classifiers to get very strong classifier
  - Weak classifier – slightly better than random on training data
  - Resulting very strong classifier – can get zero training error
- AdaBoost algorithm
- Boosting v. Logistic Regression
  - Both linear model, boosting "learns" features
  - 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