Ensembles. Stacked generalization. AdaBoost

Evgeny Burnaev

Skoltech, Moscow, Russia

Outline

- A predictor, feature $\mathbf{x} \in \mathbb{R}^d$ has distribution D
- $f(\mathbf{x})$ is a deterministic function from some concept class
- **Goal**:
  - Based on m training pairs $\{(\mathbf{x}_i, y_i = f(\mathbf{x}_i))\}_{i=1}^m$ drawn i.i.d. from D produce a classifier $\widehat{f}(\mathbf{x}) \in \{0, 1\}$
  - Choose $\widehat{f}$ to have low generalization error $R(\widehat{f}) = \mathbb{E}_D \left[1_{\widehat{f}(\mathbf{x}) \neq f(\mathbf{x})} \right]$

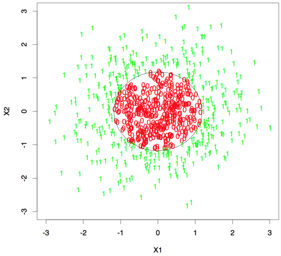
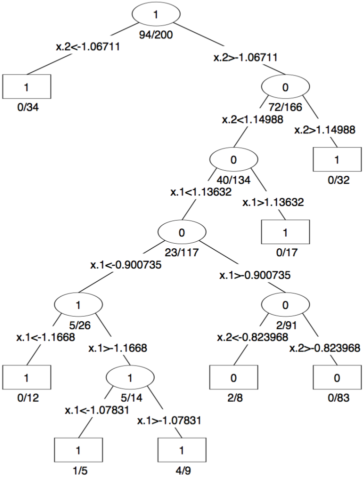
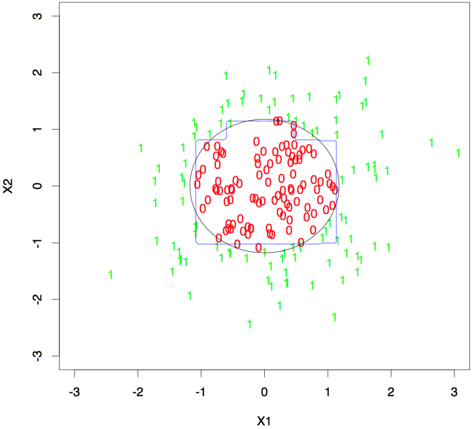


Figure – “Sphere” in $\mathbb{R}^{10}$

Sample of size 200



Sample of size 200



In case of "Sphere" in $\mathbb{R}^{10}$ CART produces a rather noisy and inaccurate rule $\widehat{f}(\mathbf{x})$, with error rates around 30%

Ensemble of classifiers

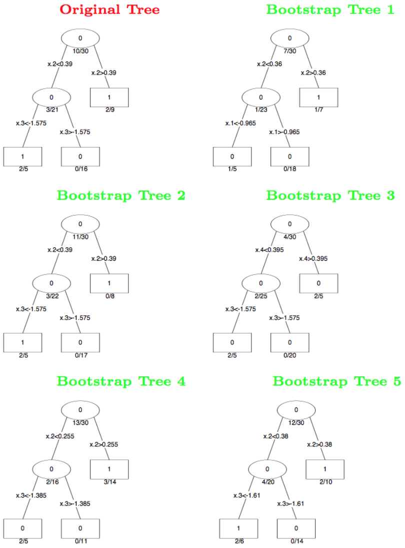
- For simplicity we consider a binary classification problem. Let us denote by $h_1(\mathbf{x}), \dots, h_T(\mathbf{x})$ some binary classifiers
- Typical ensembling procedure has the form
  - Simple voting:
$$H(h_1(\mathbf{x}), \dots, h_T(\mathbf{x})) = \frac{1}{T}\sum_{t=1}^{T} h_t(\mathbf{x}),$$
  - Weighted voting:
$$H(h_1(\mathbf{x}), \dots, h_T(\mathbf{x})) = \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}),$$
  - Mixture of experts
$$H(h_1(\mathbf{x}), \dots, h_T(\mathbf{x})) = \sum_{t=1}^{T} g_t(\mathbf{x}) h_t(\mathbf{x})$$
- Final decision
$$f_T(\mathbf{x}) = \mathrm{sign}\{H(h_1(\mathbf{x}), \dots, h_T(\mathbf{x}))\}$$

- Bagging or "bootstrap averaging" averages a given procedure over many samples to reduce its variance
- Let us denote by
  - $S_m = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$ a sample of size m
  - $\widehat{h}_S(\mathbf{x})$ a classifier, such as a tree, trained using the sample S
- To bag $\widehat{f}$ we draw bootstrap samples $S^{*,1}, \ldots, S^{*,B}$ each of size m with replacement from the training data
- In each bootstrap sample $S^{*,1}, \ldots, S^{*,B}$ we use only subset of randomly selected features
- We train classifiers $\widehat{h}_{S^{*,b}}(\mathbf{x})$ on each of $S^{*,b}$, $b = 1, \ldots, B$
- Then

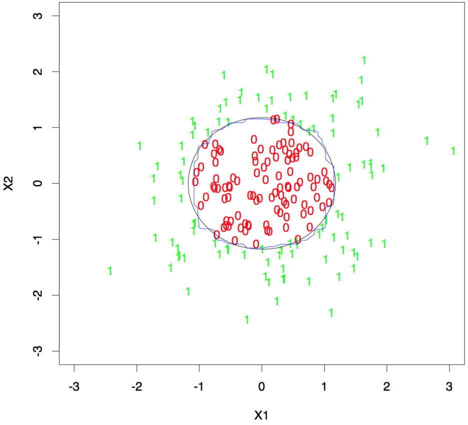
$$\widehat{f}_{\text{bag}}(\mathbf{x}) = \text{MajorityVote}\left\{\left(\widehat{h}_{S^{*,b}}(\mathbf{x})\right)_{b=1}^{B}\right\}$$

- Bagging can dramatically reduce the variance of unstable procedures (like trees), leading to improved prediction
- However any simple structure in h (e.g. a tree) is lost

Example: Bagging

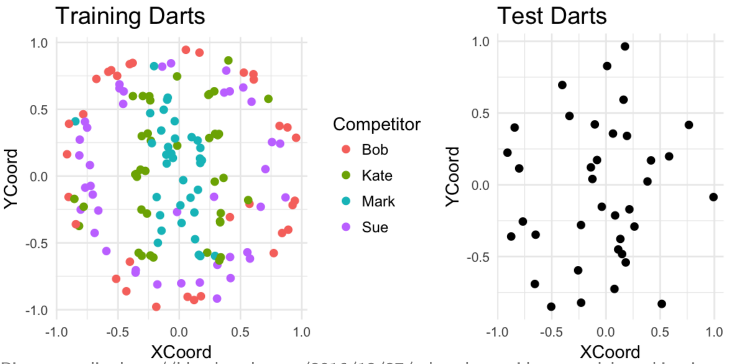


Decision Boundary: Bagging



"Sphere" in $\mathbb{R}^{10}$: Bagging averages many trees, and produces smoother decision boundaries

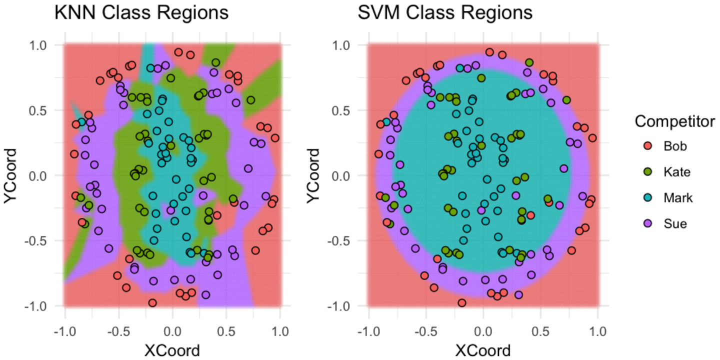
Stacking motivation: the game of Darts



Picture credit: http://blog.kaggle.com/2016/12/27/a-kagglers-guide-to-model-stacking-in-practice

- Select k nearest neighbours as base model 1
- Fit base model 1 in the most fancy way possible
  (grid search for optimal k using K-fold cross-validation, etc.)
- k-NN accuracy on Test Darts: 70%

- Select Support Vector Machine as base model 2
- Fit base model 2 in the most fancy way possible
  (different penalizations, grid search for optimal kernel width using K-fold cross-validation, etc.)
- SVM accuracy on Test Darts: 78%



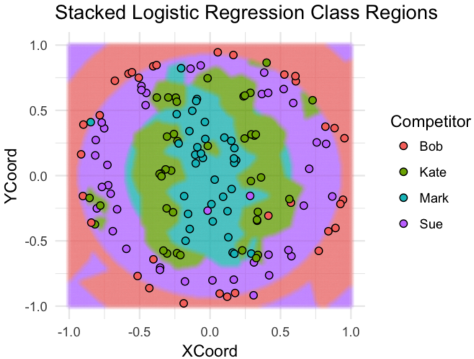
Picture credit: http://blog.kaggle.com/2016/12/27/a-kagglers-guide-to-model-stacking-in-practice

Stacked generalization aka stacking: blend output of weak learners (weak signals) with raw features

Stacking base models

1. Partition `train` into 5 folds
2. Create `train_meta`/`test_meta`: same `row/fold Ids` as in `train`/`test`, empty `M1`/`M2`
3. For each $\mathrm{Fold}_i \in \{\text{Fold}_1, \dots, \text{Fold}_5\}$
   - Combine the other 4 folds for training $\to \mathrm{Fold}_{-i}$
   - Fit each base model to Fold_{-i}, predict on Fold_i, save predictions to `M1`/`M2` in `train_meta`
4. Fit each base model to `train`, predict on `test`, save predictions to `M1`/`M2` in `test_meta`
5. Fit stacking model `F` to `train_meta`, using `M1`/`M2` as features
6. Use the stacked model `F` to make final predictions on `test_meta`

Results for base models



Picture credit: http://blog.kaggle.com/2016/12/27/a-kagglers-guide-to-model-stacking-in-practice

- Bootstrapping: a general statistical technique for computing sample functionals (and their variance)
- Bagging: meta-learner over arbitrary weak algorithms via **b**ootstrap **agg**regation
- The Random Forest algorithm: bagging over decision trees
- Stacked generalization aka stacking: blend output of weak learners (weak signals) with raw features

- **problem**: filter out spam (junk email)
- gather large collection of examples of spam and non-spam

From: yoav@att.com	Rob, can you review a paper...	non-spam
From: xa412@hotmail.com	Earn money without working!!!! ...	spam
⋮	⋮	⋮

- **goal**: get computer learn from examples to distinguish spam from non-spam
- **main observation**:
  - easy to find "rules of thumb" that are "often" correct

    if 'v1agr@' occurs in message, then predict "spam"
  - hard to find single rule that is very highly accurate

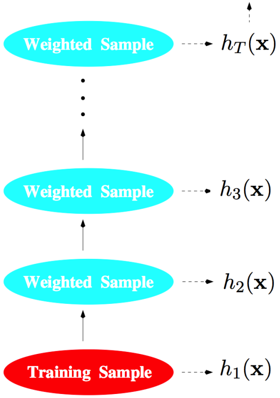
The Boosting Approach I

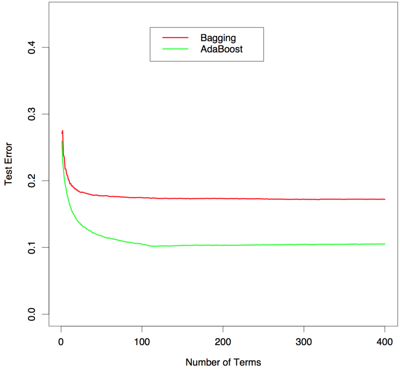
- devise computer program for deriving rough rules of thumb
- apply procedure to subset of emails
- obtain rule of thumb
- apply to 2nd subset of emails
- obtain 2nd rule of thumb
- repeat T times
- aggregate

Final Classifier

$$f_T(\mathbf{x}) = \text{sign}\left[\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})\right]$$

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





- 2000 points, "Sphere" in $\mathbb{R}^{10}$; Bayes error rate is 0%
- Trees are grown Best First without pruning
- Leftmost iteration is a single tree

- We consider a binary classification with $Y = \{-1, +1\}$
- As a strong classifier we consider weighted voting scheme, i.e.

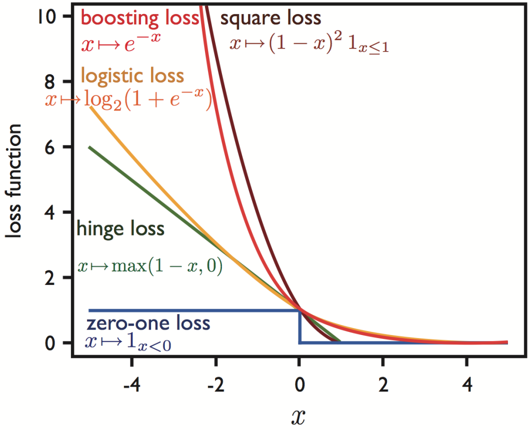
$$\widehat{f}_T(\mathbf{x}) = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})\right)$$

- As a risk we consider accuracy, i.e.

$$\widehat{R}(f_T) = \frac{1}{m}\sum_{i=1}^{m} 1\left\{y_i \cdot \left[\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}_i)\right] \leq 0\right\}$$

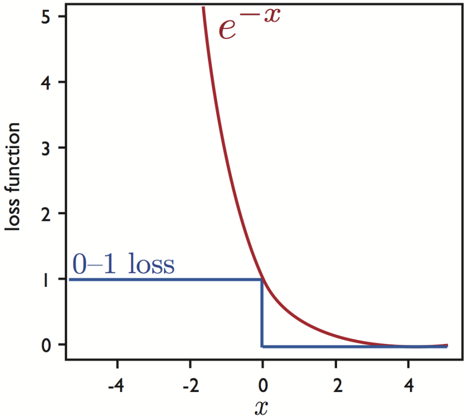
- Two main heuristics, underlying boosting
  - We fix $\alpha_1 h_1(\mathbf{x}), \ldots, \alpha_{t-1} h_{t-1}(\mathbf{x})$ when adding $\alpha_t h_t(\mathbf{x})$
  - We use continuous upper bound for accuracy

- Examples of several convex upper bounds on the zero-one loss



Exponential upper bound for binary objective function

- Objective Function: convex and differentiable



- Since $1_{z \le 0} \le e^{-z}$, we get that

$$1_{\left\{y_i \cdot \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}_i) \le 0\right\}} \le \exp\left(-y_i \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}_i)\right)$$

- Let us consider an upper bound for $\widehat{R}(f)$

$$\widehat{R}(f_T) = \frac{1}{m} \sum_{i=1}^{m} 1_{\left\{y_i \cdot \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}_i) \le 0\right\}} \le$$

$$\le \widetilde{R}(f_T) = \frac{1}{m} \sum_{i=1}^{m} \exp\left(-y_i \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}_i)\right)$$

- We will optimize $\widehat{R}(f_T)$ w.r.t. a new weak classifier $h_T(\mathbf{x})$ and its weight α_T given that $\{\alpha_t, h_t(\mathbf{x})\}_{t=1}^{T-1}$ are fixed

- Let us denote

$$w_{i,T-1} = \exp\left(-y_i \sum_{t=1}^{T-1} \alpha_t h_t(\mathbf{x}_i)\right)$$

$$\widetilde{w}_{i,T} = \frac{w_{i,T-1}}{\sum_j w_{j,T-1}}$$

- Then

$$\widetilde{R}(f_{T-1}) = \frac{1}{m} \sum_{i=1}^{m} \underbrace{\exp\left(-y_i \sum_{t=1}^{T-1} \alpha_t h_t(\mathbf{x}_i)\right)}_{w_{i,T-1}} =$$

$$= \frac{1}{m} \sum_{i=1}^{m} w_{i,T-1}$$

Let us re-write an upper bound $\widetilde{R}(f)$

$$\widetilde{R}(f_T) = \frac{1}{m}\sum_{i=1}^{m}\underbrace{\exp\left(-y_i\sum_{t=1}^{T}\alpha_t h_t(\mathbf{x}_i)\right)}_{w_{i,T}} =$$

$$= \frac{1}{m}\sum_{i=1}^{m}\underbrace{\exp\left(-y_i\sum_{t=1}^{T-1}\alpha_t h_t(\mathbf{x}_i)\right)}_{w_{i,T-1}}\exp(-y_i\alpha_T h_T(\mathbf{x}_i))$$

$$= \frac{1}{m}\sum_{i=1}^{m} w_{i,T-1}\exp(-y_i\alpha_T h_T(\mathbf{x}_i))$$

Let us re-write an upper bound $\widetilde{R}(f)$

$$
\begin{aligned}
\widetilde{R}(f_T) &= \frac{1}{m}\sum_{i=1}^{m} w_{i,T-1}\exp(-y_i\alpha_T h_T(\mathbf{x}_i)) = \\
&= \frac{1}{m}\sum_{i=1}^{m} \frac{[\sum_{k=1}^{m} w_{k,T-1}]}{[\sum_{k=1}^{m} w_{k,T-1}]} w_{i,T-1}\exp(-y_i\alpha_T h_T(\mathbf{x}_i)) = \\
&= \frac{1}{m}\left[\sum_{k=1}^{m} w_{k,T-1}\right]\sum_{i=1}^{m} \frac{w_{i,T-1}}{[\sum_{k=1}^{m} w_{k,T-1}]}\exp(-y_i\alpha_T h_T(\mathbf{x}_i)) = \\
&= \underbrace{\frac{1}{m}\sum_{k=1}^{m} w_{k,T-1}}_{\widetilde{R}(f_{T-1})} \cdot \sum_{i=1}^{m} \widetilde{w}_{i,T}\exp(-y_i\alpha_T h_T(\mathbf{x}_i)) = \\
&= \widetilde{R}(f_{T-1}) \cdot \sum_{i=1}^{m} \widetilde{w}_{i,T} e^{-y_i\alpha_T h_T(\mathbf{x}_i)}
\end{aligned}
$$

- Upper bound $\widetilde{R}(f_{T-1})$ is fixed from the previous boosting step
- Let us optimize an upper bound for $\widehat{R}(f)$

$$\widehat{R}(f_T) \leq \widetilde{R}(f_{T-1}) \cdot \sum_{i=1}^{m} \widetilde{w}_{i,T} \exp(-y_i \alpha_T h_T(\mathbf{x}_i)) \to \min_{\alpha_T, h_T(\cdot)},$$

i.e. we tune only the weak classifier $h_T(\cdot)$ and its weight α_T

- An upper bound for $\widehat{R}(f)$

$$\widehat{R}(f_T) \leq \widetilde{R}(f_{T-1}) \cdot \sum_{i=1}^{m} \widetilde{w}_{i,T} \exp(-y_i \alpha_T h_T(\mathbf{x}_i)) \to \min_{\alpha_T, h_T(\cdot)}$$

- For $\widetilde{\mathbf{w}}_T = (\widetilde{w}_{1,T}, \ldots, \widetilde{w}_{m,T})$ we define a weighted classification error

$$N_T = N(h_T, \widetilde{\mathbf{w}}_T) = \sum_{i=1}^{m} \widetilde{w}_{i,T} \cdot 1_{\{y_i \cdot h_T(\mathbf{x}_i) \leq 0\}}, \; P_T = 1 - N_T,$$

- Since for the weak learner $y_i \cdot h_T(\mathbf{x}_i) \in \{-1, +1\}$, then

$$\sum_{i=1}^{m} \widetilde{w}_{i,T} \exp(-y_i \alpha_T h_T(\mathbf{x}_i)) =$$

$$= \sum_{i: y_i \cdot h_T(\mathbf{x}_i) = -1} \widetilde{w}_{i,T} \exp(\alpha_T) + \sum_{i: y_i \cdot h_T(\mathbf{x}_i) = +1} \widetilde{w}_{i,T} \exp(-\alpha_T) =$$

$$= N_T \exp(\alpha_T) + (1 - N_T) \exp(-\alpha_T)$$

- We get that

$$\widehat{R}(f_T) \leq \widetilde{R}(f_{T-1}) \cdot \left(e^{-\alpha_T} (1 - N_T) + e^{\alpha_T} N_T \right) \to \min_{\alpha_T, h_T(\cdot)}$$

- We proved that

$$\widehat{R}(f_T) \leq \widetilde{R}(f_{T-1}) \cdot \left(e^{-\alpha_T}(1 - N_T) + e^{\alpha_T} N_T\right) \to \min_{\alpha_T, h_T(\cdot)}$$

- Let us fix $h_T(\cdot)$. Then optimal α_T is equal to

$$\alpha_T^* = \arg\min_{\alpha_T} \left(e^{-\alpha_T}(1 - N_T) + e^{\alpha_T} N_T\right) =$$
$$= \frac{1}{2} \log \frac{P_T}{N_T} = \frac{1}{2} \log \frac{1 - N_T(h_T, \widetilde{\mathbf{w}}_T)}{N_T(h_T, \widetilde{\mathbf{w}}_T)}$$

- For optimal α_T^* we get that

$$\begin{aligned}\widehat{R}(f_T) &\leq \widetilde{R}(f_{T-1}) \cdot \left(e^{-\alpha_T^*}(1 - N_T) + e^{\alpha_T^*} N_T\right) \\ &\leq \widetilde{R}(f_{T-1}) \cdot \left(1 - \left(\sqrt{P_T} - \sqrt{N_T}\right)^2\right) \to \min_{h_T(\cdot)}\end{aligned}$$

- Then optimal $h_T(\cdot)$ is given by

$$h_T^*(\cdot) = \arg\max_{h_T(\cdot)} \left(\sqrt{P_T(h_T, \widetilde{\mathbf{w}}_T)} - \sqrt{N_T(h_T, \widetilde{\mathbf{w}}_T)}\right)^2$$

- Let us assume that $h_T(\cdot)$ is weak learnable, i.e. we can find $h_T(\cdot)$ such that $N_T < P_T = 1 - N_T$

- For $N_T < P_T = 1 - N_T$ the problem

$$h_T^*(\cdot) = \arg\max_{h_T(\cdot)} \left(\sqrt{P_T(h_T, \widetilde{\mathbf{w}}_T)} - \sqrt{N_T(h_T, \widetilde{\mathbf{w}}_T)}\right)^2$$

  reduces to

- The problem

$$h_T^*(\cdot) = \arg\max_{h(\cdot)} \left\{\sqrt{P_T} - \sqrt{N_T}\right\} = \arg\min_{h(\cdot)} N_T(h, \widetilde{\mathbf{w}}_T),$$

  where
  - weighted classification error

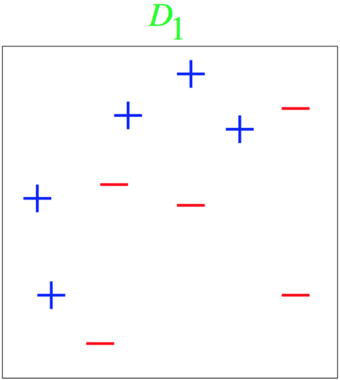
$$N_T = N(h_T, \widetilde{\mathbf{w}}_T) = \sum_{i=1}^{m} \widetilde{w}_{i,T} 1_{\{y_i \cdot h_T(\mathbf{x}_i) \le 0\}}$$

  - weights

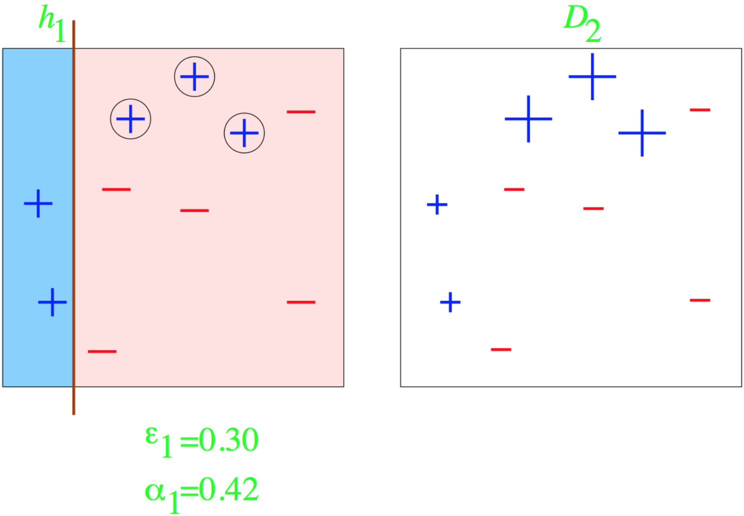
$$w_{i,T-1} = \exp\left(-y_i f_{T-1}(\mathbf{x}_i)\right),\ \ \widetilde{w}_{i,T} = \frac{w_{i,T-1}}{\sum_j w_{j,T-1}}$$

AdaBoost$(S_m = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\})$

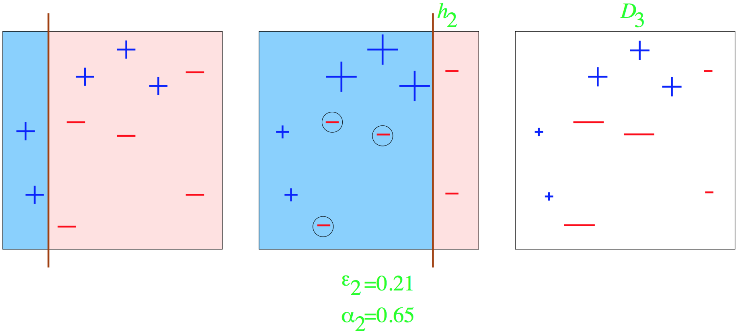
1. **for** $i \leftarrow 1$ **to** m **do**
2. $\quad w_{i,1} \leftarrow \frac{1}{m}$
3. **for** $t \leftarrow 1$ **to** T **do**
4. $\quad$ Learn a based classifier:
   $h_t \leftarrow$ base classif. with small $N(h_t, \widetilde{\mathbf{w}}_t) = \sum_{i=1}^m \widetilde{w}_{i,t} 1_{\{y_i \cdot h_t(\mathbf{x}_i) \leq 0\}}$
5. $\quad \alpha_t \leftarrow \frac{1}{2} \log \frac{1 - N(h_t, \widetilde{\mathbf{w}}_t)}{N(h_t, \widetilde{\mathbf{w}}_t)}$
7. $\quad$ **for** $i \leftarrow 1$ **to** m **do**
8. $\quad\quad w_{i,t+1} \leftarrow w_{i,t} \exp(-\alpha_t y_t h_t(\mathbf{x}_i))$
9. $\quad\quad \widetilde{w}_{i,t+1} \leftarrow \frac{w_{i,t+1}}{\sum_{j=1}^m w_{j,t+1}}$
10. $\quad f_t \leftarrow \sum_{s=1}^t \alpha_s h_s$
10. **return** $\widehat{f}_T = \mathrm{sign}(f_T)$



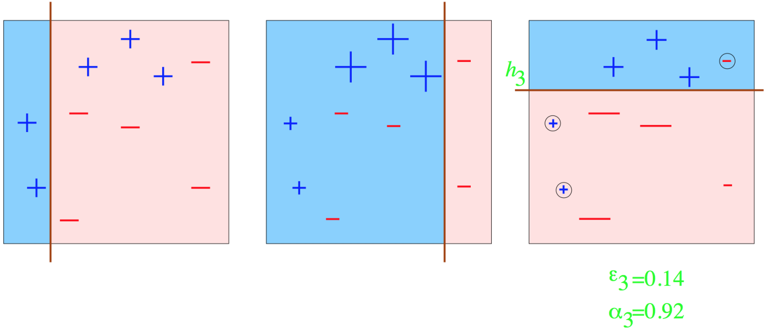
Weak classifiers = vertical or horizontal half-planes


h_1
D_2
$\varepsilon_1 = 0.30$
$\alpha_1 = 0.42$

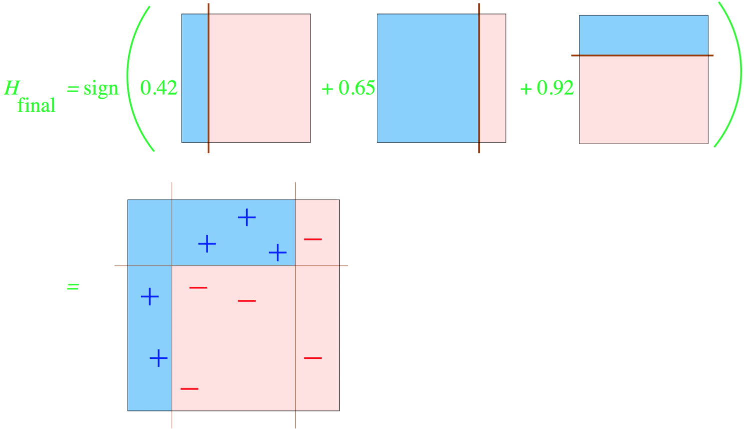
Toy Example: Round 2



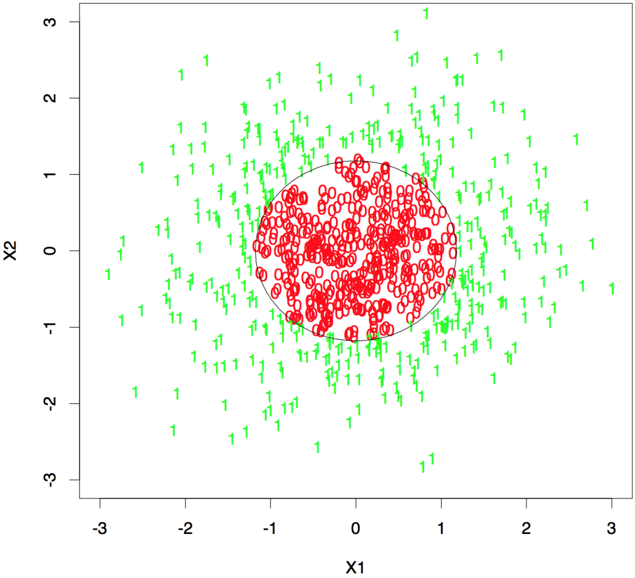
Toy Example: Round 3



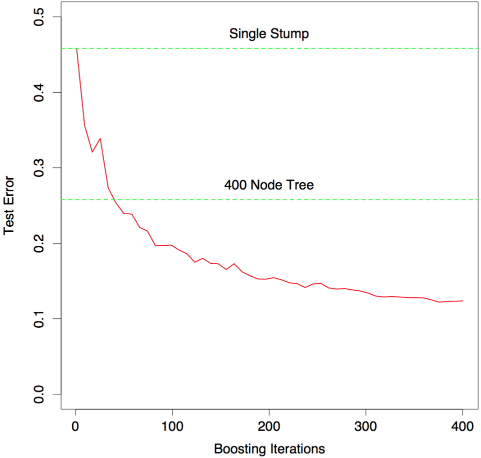
Toy Example: Final Classifier



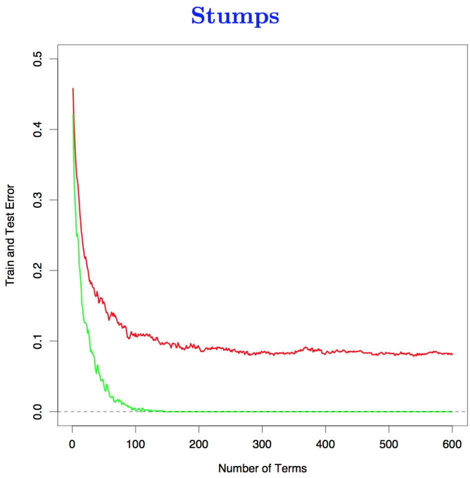
Example: "Sphere" in $\mathbb{R}^{10}$



Boosting Stumps



“Sphere” in $\mathbb{R}^{10}$: A stump is a two-node tree, after a single split. Boosting stumps works remarkably well on this problem



"Sphere" in $\mathbb{R}^{10}$: Boosting drives the training error to zero. Further iterations continue to improve test error in many examples

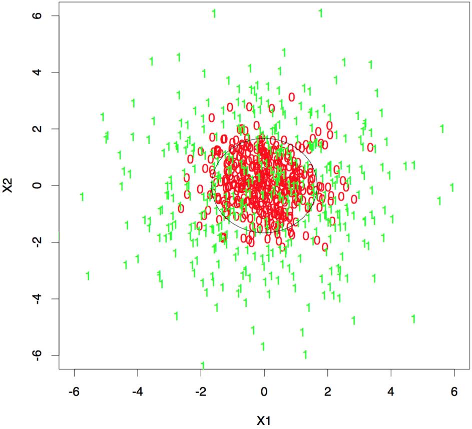
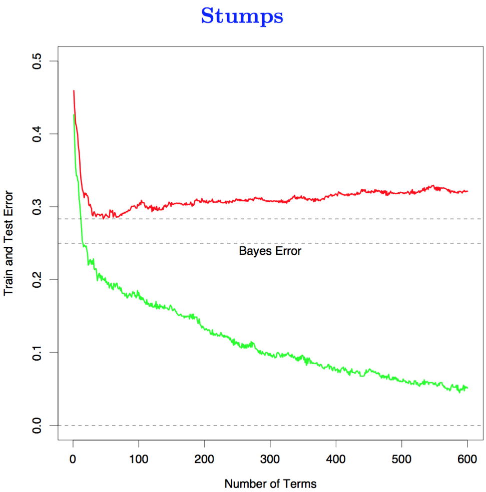


Figure – "Gaussians" in $\mathbb{R}^{10}$. Bayes error is 25%

Boosting Noisy Problems II



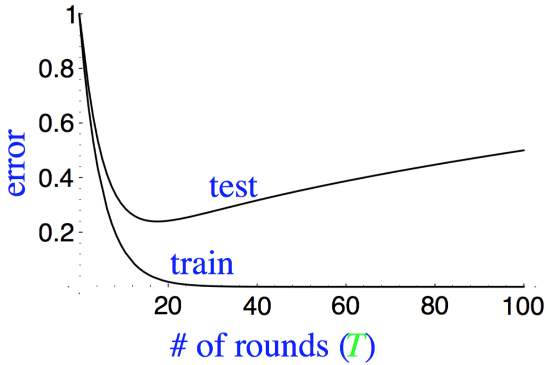
"Gaussians" in $\mathbb{R}^{10}$. Bayes error is 25%. Here the test error does increase, but quite slowly

[Video: AdaBoost in Action]
https://www.youtube.com/watch?v=k4G2VCuOMMg

- **Base Learners**: decision trees, quite often just decision stumps (trees of depth one)
- Boosting stumps
  - data in $\mathbb{R}^d$, e.g. $d = 2$ (height$(\mathbf{x})$, weight$(\mathbf{x})$)
  - associate a stump to each component
  - pre-sort each component: $O(dm \log m)$
  - at each round, find best component and threshold
  - total complexity: $O((m \log m)N + mdT)$
  - stumps are not weak learners (XOR problem)
- For SVM boosting usually is not effective
- Additional stopping criterion: error increase on a separate validation set

- AdaBoost assigns larger weights to harder examples
- Applications:
  - Detecting mislabeled examples
  - Dealing with noisy data: regularization based on the average weight assigned to a point (soft margin idea for boosting)

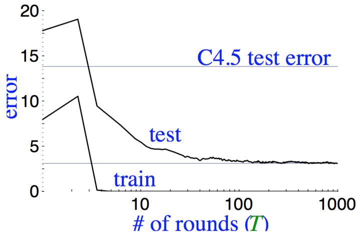
How will Test Error Behave? (A First Guess)



Expect:

- training error to continue to drop (or reach zero)
- test error to increase when h_{final} becomes "too complex"
  - "Occam's razor"
  - overfitting: hard to know when to stop training

Empirical Observations



(boosting C4.5 on "letter" dataset)

Expect:

- 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!

	# rounds		
	5	100	1000
train error	0.0	0.0	0.0
test error	8.4	3.3	3.1

- Occam's razor wrongly predicts "simpler" rule is better

- Bias: not made any worse by bagging multiple hypotheses

$$\mathbb{E}_{\mathbf{x},y}\Big[\Big(\mathbb{E}_{S_m}\Big[\frac{1}{T}\sum_{t=1}^{T}h_t(\mathbf{x}|S_m)\Big]-\mathbb{E}[y|\mathbf{x}]\Big)^2\Big]=$$

$$=\mathbb{E}_{\mathbf{x},y}\Big[\Big(\frac{1}{T}\sum_{t=1}^{T}\mathbb{E}_{S_m}[h_t(\mathbf{x}|S_m)]-\mathbb{E}[y|\mathbf{x}]\Big)^2\Big]=$$

$$=\mathbb{E}_{\mathbf{x},y}\Big[\big(\mathbb{E}_{S_m}\big[h(\mathbf{x}|S_m)\big]-\mathbb{E}[y|\mathbf{x}]\big)^2\Big]$$

- Variance: T times lower for uncorrelated hypotheses, yet not as much an improvement for highly correlated

$$\mathbb{E}_{\mathbf{x},y}\Big[\mathbb{E}_{S_m}\Big[\Big(\frac{1}{T}\sum_{t=1}^{T} h_t(\mathbf{x}|S_m) - \mathbb{E}_{S_m}\Big[\frac{1}{T}\sum_{t=1}^{T} h_t(\mathbf{x}|S_m)\Big]\Big)^2\Big]\Big] =$$

$$= \frac{1}{T}\mathbb{E}_{\mathbf{x},y}\Big[\mathbb{E}_{S_m}\Big[\Big(h(\mathbf{x}|S_m) - \mathbb{E}_{S_m}\big[h(\mathbf{x}|S_m)\big]\Big)^2\Big]\Big] +$$

$$+ \frac{T(T-1)}{T^2}\mathbb{E}_{\mathbf{x},y}\Big[\mathbb{E}_{S_m}\Big[\Big(h(\mathbf{x}|S_m) - \mathbb{E}_{S_m}\big[h(\mathbf{x}|S_m)\big]\Big)\times$$

$$\times \Big(\widetilde{h}(\mathbf{x}|S_m) - \mathbb{E}_{S_m}\big[\widetilde{h}(\mathbf{x}|S_m)\big]\Big)\Big]\Big]$$