

Margin-Based Generalization Lower Bounds for Boosted Classifiers

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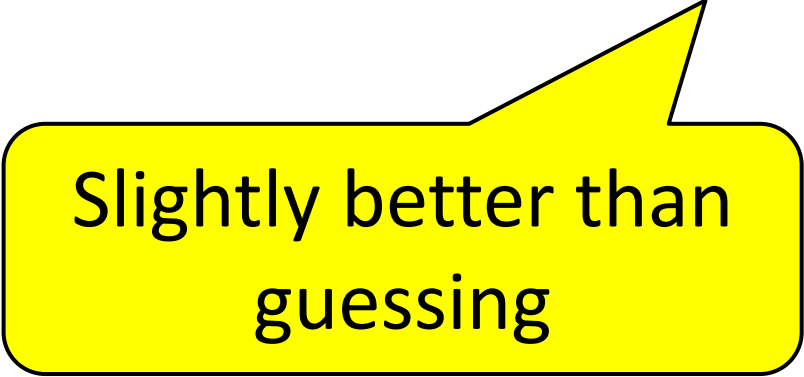


Boosting Algorithms

- Construct strong classifiers out of weak ones.



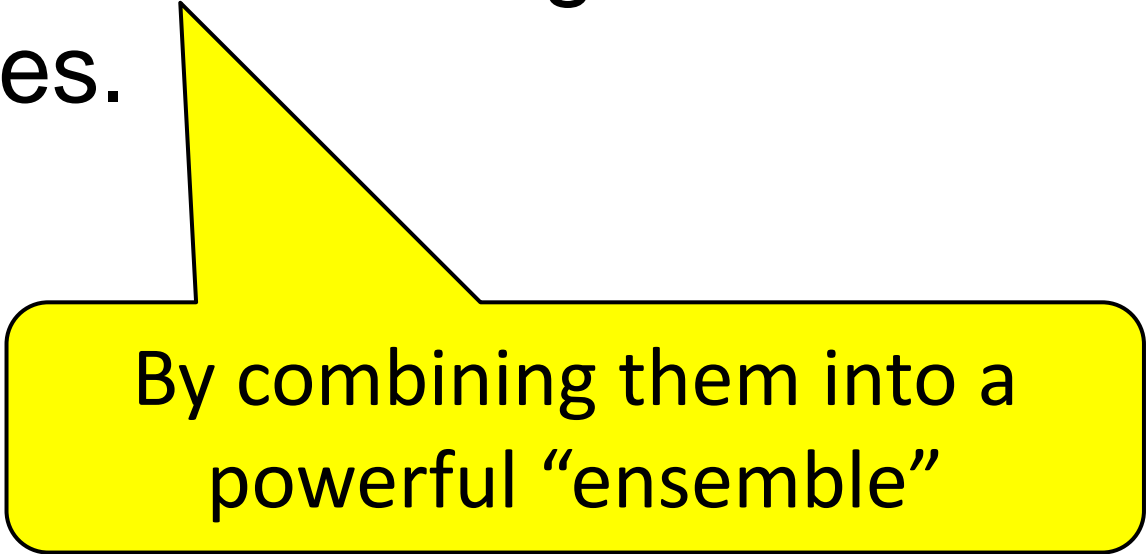
Accurate



Slightly better than
guessing

Boosting Algorithms

- Construct strong classifiers out of weak ones.



By combining them into a powerful “ensemble”

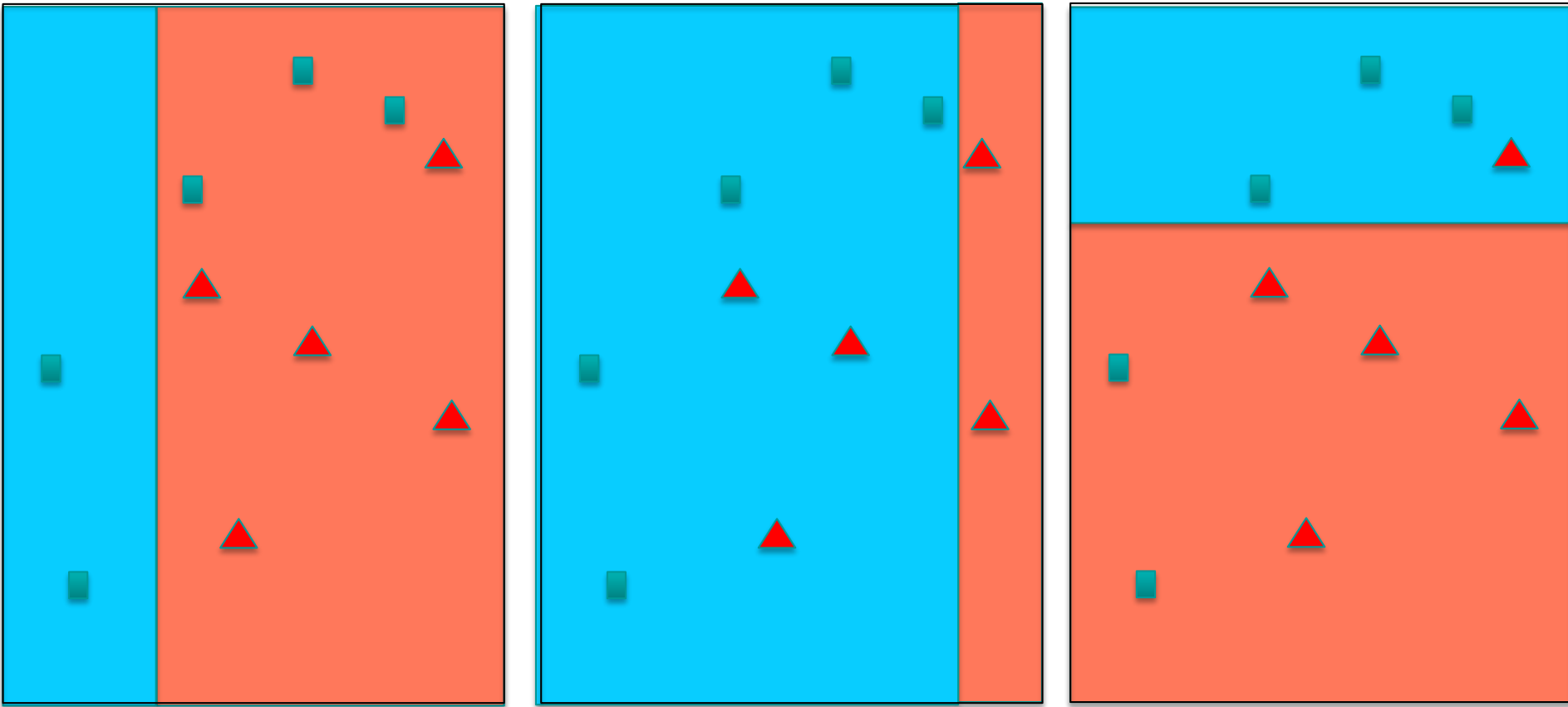
Boosting Algorithms

- Construct strong classifiers out of weak ones.
- Intuition: Train many weak classifiers, each “focusing” on a different part of the input space.

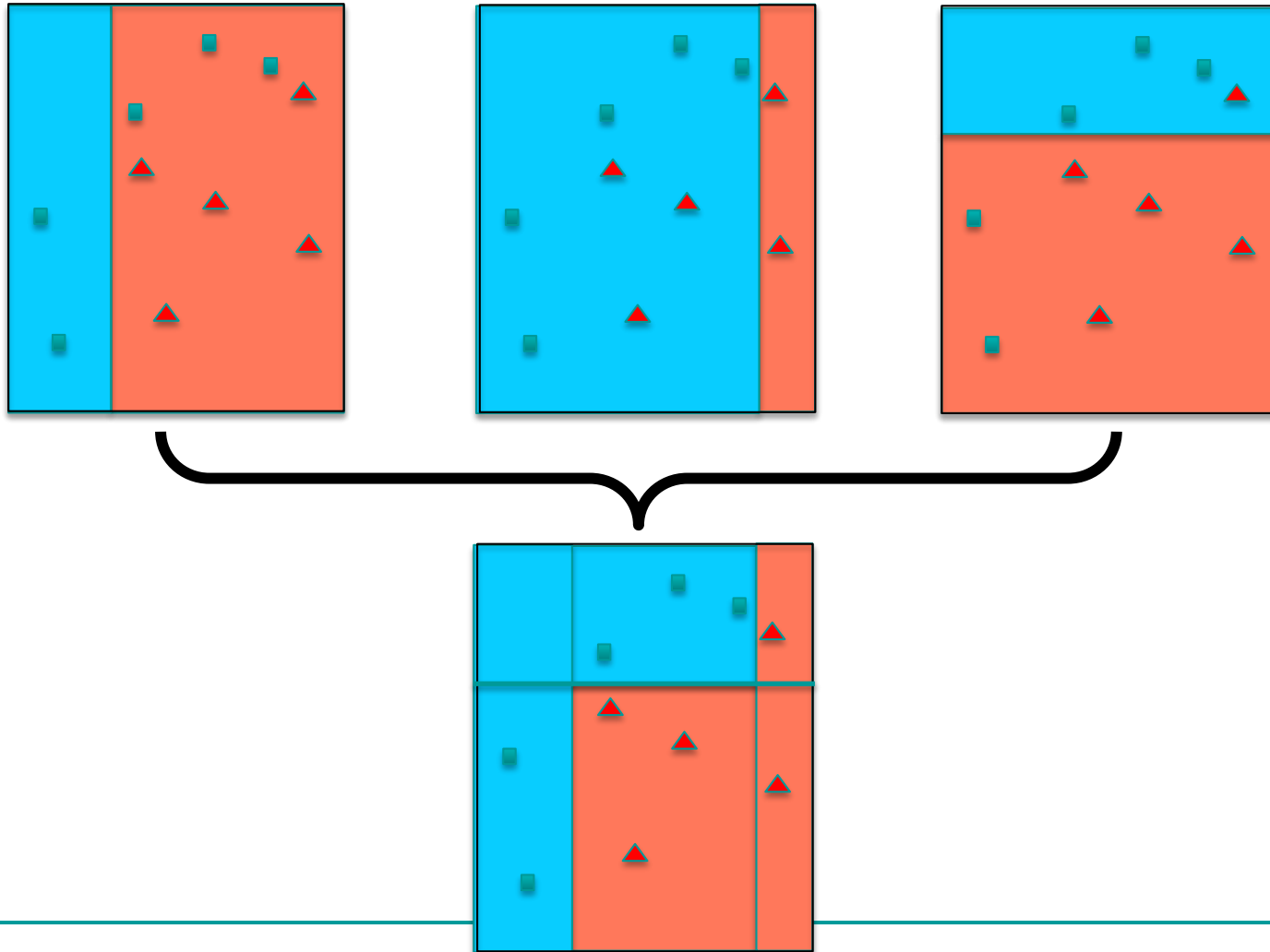


Achieved by re-weighting
the input sample

Example : Axis Aligned Lines



Example : Axis Aligned Lines



Boosting Algorithms and Margins

- Surprising phenomenon : Even though the strong classifier gets more complicated, it does not overfit.

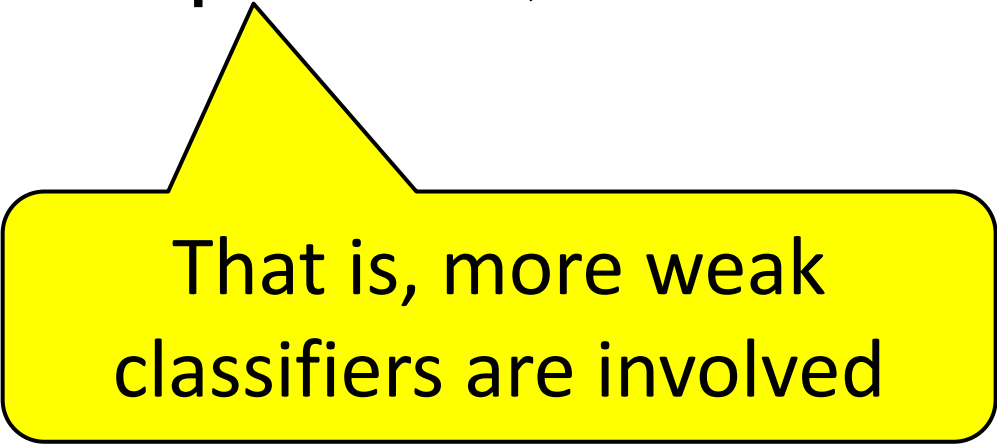
Boosting Algorithms and Margins

- Surprising phenomenon : Even though the strong classifier gets more complicated, it performs better.

Observed in experiments
by Schapire *et al.*

Boosting Algorithms and Margins

- Surprising phenomenon : Even though the strong classifier gets more complicated, it does not overfit.



That is, more weak classifiers are involved

Boosting Algorithms and Margins

- Surprising phenomenon : Even though the strong classifier gets more complicated, it does not overfit.
- Prominent explanation : Margin Theory

Loosely speaking, the “confidence” of the classifier on a point.

Margin Theory

- Formally, let $\mathcal{H} \subseteq \mathcal{X} \rightarrow \{-1, 1\}$ be the space of weak classifiers, and $S = \{(x_j, y_j)\}_{j=1}^m$ is the sample used to train a strong classifier $f = \sum_{h \in \mathcal{H}} \alpha_h h$.
- The margin of f on the j^{th} sample point is defined as $\theta_j := y_j f(x_j)$

Margin Theory

- Formally, let $\mathcal{H} \subseteq \mathcal{X} \rightarrow \{-1, 1\}$ be the space of weak classifiers, and $S = \{(x_j, y_j)\}_{j=1}^m$ is the sample used to train a strong classifier $f = \sum_{h \in \mathcal{H}} \alpha_h h$.
- The margin of a point is defined as $\max_{h \in \mathcal{H}} y_j h(x_j)$.
A convex combination of weak classifiers.

Margin Theory

- Formally, let $\mathcal{H} \subseteq \mathcal{X} \rightarrow \{-1, 1\}$ be the space of weak classifiers, and $S = \{(x_j, y_j)\}_{j=1}^m$ is the sample used to train a strong classifier $f = \sum_{h \in \mathcal{H}} \alpha_h h$.
- The margin of f is called a voting-classifier point is defined as $\theta_j := y_j f(x_j)$

Margin Theory

- Formally, let $\mathcal{H} \subseteq \mathcal{X} \rightarrow \{-1, 1\}$ be the space of weak classifiers, and $S = \{(x_j, y_j)\}_{j=1}^m$ is the sample used to train. If θ_j is positive, then $\text{sign}(f)$ classifies (x_j, y_j) correctly. $f = \sum_{h \in \mathcal{H}} \alpha_h h$.
- The margin of f on the j^{th} sample point is defined as $\theta_j := y_j f(x_j)$

Margin Theory

- Formally, let $\mathcal{H} \subseteq \mathcal{X} \rightarrow \{-1, 1\}$ be the space of weak classifiers, and $S = \{(x_j, y_j)\}_{j=1}^m$ is the sample used to train f .
Intuitively, the closer θ_j is to 1, the more “confident” f is. $\alpha_h h$.
- The margin of f on the j^{th} sample point is defined as $\theta_j := y_j f(x_j)$

Margin-Based *Upper* Bounds

- Schapire *et al.* (1998) showed the following bound on the error probability of voting classifiers.

$$\Pr_{(x,y) \sim \mathcal{D}}[yf(x) \leq 0] \leq \Pr_{(x,y) \sim \mathcal{S}}[yf(x) \leq \theta] + O\left(\sqrt{\frac{\ln|\mathcal{H}| \ln m}{m\theta^2}}\right)$$

Margin-Based *Upper* Bounds

- Schapire *et al.* (1998) showed the following bound on the error probability of voting classifiers.

$$\Pr_{(x,y) \sim \mathcal{D}} [yf(x) \leq 0]$$

The error probability of f with respect to the unknown distribution \mathcal{D} over $\mathcal{X} \times \{-1,1\}$.

$$\left(\frac{|\mathcal{H}| \ln m}{m\theta^2} \right)$$

Margin-Based *Upper* Bounds

- Schapire *et al.* (1998) showed the following bound on the error probability of voting classifiers.

The fraction of sample points with margin at most θ .

$$\Pr_{(x,y) \sim \mathcal{D}} [yf(x) \leq \theta] \leq \Pr_{(x,y) \sim \mathcal{S}} [yf(x) \leq \theta] + O \left(\sqrt{\frac{\ln |\mathcal{H}| \ln m}{m\theta^2}} \right)$$

Margin-Based *Upper* Bounds

- Schapire *et al.* (1998) showed the following relationship between the performance of voting classifiers and the margin of the weak classifier.

Holds for all voting classifiers f and margins $\theta \in (0,1]$

$$\Pr_{(x,y) \sim \mathcal{D}} [yf(x) \leq 0]$$

$$\leq \Pr_{(x,y) \sim \mathcal{S}} [yf(x) \leq \theta] + O \left(\sqrt{\frac{\ln |\mathcal{H}| \ln m}{m\theta^2}} \right)$$

Margin-Based Upper Bounds

This holds with high probability over the choice of the m sample points

forall classifiers.

$$\Pr_{(x,y) \sim \mathcal{D}} [f(x) \leq 0]$$

$$\leq \Pr_{(x,y) \sim S} [yf(x) \leq \theta] + O \left(\sqrt{\frac{\ln |\mathcal{H}| \ln m}{m\theta^2}} \right)$$

Margin-Based *Upper* Bounds

- Schapire following voting classifiers

The result gave rise to boosting algorithms that intentionally aim to optimize margins

$$\Pr_{(x,y) \sim \mathcal{D}} [yf(x) \leq 0]$$

$$\leq \Pr_{(x,y) \sim \mathcal{S}} [yf(x) \leq \theta] + O\left(\sqrt{\frac{\ln |\mathcal{H}| \ln m}{m\theta^2}}\right)$$

Margin-Based *Upper* Bounds

- Breimann (1999) showed the following bound on the error probability of voting classifiers.

$$\Pr_{(x,y) \sim \mathcal{D}} [yf(x) \leq 0] \leq O\left(\frac{\ln|\mathcal{H}| \ln m}{m\hat{\theta}^2}\right)$$

Holds for all voting classifiers f
where $\hat{\theta}$ is the minimum margin

Margin-Based *Upper* Bounds

- Breiman's bound on the error of voting classifiers

This holds with high probability over the choice of the m sample points

$$\Pr_{(x,y) \sim \mathcal{D}} [yf(x) \leq 0] \leq O\left(\frac{\ln|\mathcal{H}| \ln m}{m\hat{\theta}^2}\right)$$

Holds for all voting classifiers f where $\hat{\theta}$ is the minimum margin

Margin-Based *Upper* Bounds

- State-of-the-Art bounds were given by Gao and Zhou (2013)

$$\Pr_{(x,y) \sim \mathcal{D}}[yf(x) \leq 0] \leq \Pr_{(x,y) \sim \mathcal{S}}[yf(x) \leq \theta] + O\left(\frac{\ln|\mathcal{H}| \ln m}{m\theta^2} + \sqrt{\frac{\ln|\mathcal{H}| \ln m}{m\theta^2} \Pr_{(x,y) \sim \mathcal{S}}[yf(x) \leq \theta]}\right)$$

Margin-Based Upper Bounds

This holds with high probability over the choice of the m sample points were given by

$$\Pr_{(x,y) \sim \mathcal{D}} [yf(x) \leq 0] \leq \Pr_{(x,y) \sim \mathcal{S}} [yf(x) \leq \theta] + O \left(\frac{\ln |\mathcal{H}| \ln m}{m\theta^2} + \sqrt{\frac{\ln |\mathcal{H}| \ln m}{m\theta^2} \Pr_{(x,y) \sim \mathcal{S}} [yf(x) \leq \theta]} \right)$$

Holds for all voting classifiers f and margins $\theta \in (0,1]$

Margin-Based *Lower* Bounds?

- Despite being studied for over two decades, the tightness of margin-based generalization bounds was not settled.
- In fact, no margin-based lower bounds were known.

Margin-Based *Lower* Bounds!

- Our main result shows that any algorithm *A* optimizing margins cannot do much better than the known upper bounds.

Margin-Based *Lower* Bounds

- Formally, $\forall N, \theta, \tau$ There exist a set \mathcal{X} and a hypothesis set \mathcal{H} such that for every large enough m and algorithm \mathcal{A} that optimizes margins there exists a distribution \mathcal{D} for which

$$\Pr_{(x,y) \sim \mathcal{D}} [yf_{\mathcal{A}}(x) \leq 0] \geq \Pr_{(x,y) \sim \mathcal{S}} [yf_{\mathcal{A}}(x) \leq \theta] + O \left(\frac{\ln |\mathcal{H}|}{\theta^2} + \sqrt{\frac{\ln |\mathcal{H}|}{\theta^2} \Pr_{(x,y) \sim \mathcal{S}} [yf_{\mathcal{A}}(x) \leq \theta]} \right)$$

Margin-Based *Lower* Bounds

- Formally, $\forall N, \theta, \tau$ There exist a set \mathcal{X} and a hypothesis set \mathcal{H} such that for every

Where $\theta \in \left(\frac{1}{N}, \frac{1}{40}\right)$ and $\tau \in \left[0, \frac{49}{100}\right]$ \mathcal{A} that are not too large.

distribution \mathcal{D} for which

$$\Pr_{(x,y) \sim \mathcal{D}} [yf_{\mathcal{A}}(x) \leq 0] \geq \Pr_{(x,y) \sim \mathcal{S}} [yf_{\mathcal{A}}(x) \leq \theta]$$

$$+ O \left(\frac{\ln |\mathcal{H}|}{\theta^2} + \sqrt{\frac{\ln |\mathcal{H}|}{\theta^2} \Pr_{(x,y) \sim \mathcal{S}} [yf_{\mathcal{A}}(x) \leq \theta]} \right)$$

Margin-Based *Lower* Bounds

- Formally, $\forall N, \theta, \tau$ There exist a set \mathcal{X} and a hypothesis set \mathcal{H} such that for every large enough n and algorithm \mathcal{A} that optimizes the empirical error on n samples from a distribution \mathcal{D} ,
Small set of weak classifiers,
 $\ln |\mathcal{H}| = \Theta(\ln N)$

$$\Pr_{(x,y) \sim \mathcal{D}} [y f_{\mathcal{A}}(x) \leq 0] \geq \Pr_{(x,y) \sim \mathcal{S}} [y f_{\mathcal{A}}(x) \leq \theta] + O \left(\frac{\ln |\mathcal{H}|}{\theta^2} + \sqrt{\frac{\ln |\mathcal{H}|}{\theta^2} \Pr_{(x,y) \sim \mathcal{S}} [y f_{\mathcal{A}}(x) \leq \theta]} \right)$$

Margin-Based *Lower* Bounds

- Formally, $\forall N, \theta, \tau$ There exist a set \mathcal{X} and a distribution \mathcal{D} over $\mathcal{X} \times \{-1, 1\}$ that for every large enough n algorithm \mathcal{A} that optimizes margin there exists a distribution \mathcal{D} for which

$$\Pr_{(x,y) \sim \mathcal{D}} [y f_{\mathcal{A}}(x) \leq 0] \geq \Pr_{(x,y) \sim \mathcal{S}} [y f_{\mathcal{A}}(x) \leq \theta] + O \left(\frac{\ln |\mathcal{H}|}{\theta^2} + \sqrt{\frac{\ln |\mathcal{H}|}{\theta^2} \Pr_{(x,y) \sim \mathcal{S}} [y f_{\mathcal{A}}(x) \leq \theta]} \right)$$

Margin-Based *Lower* Bounds

- Formally, $\forall N, \theta, \tau$ There exist a set \mathcal{X} and a hypothesis set \mathcal{H} such that for every large enough m and algorithm \mathcal{A} that margins there exists a distribution \mathcal{D} for which

The classifier returned by \mathcal{A} .

$$\Pr_{(x,y) \sim \mathcal{D}} [yf_{\mathcal{A}}(x) \leq 0] \geq \Pr_{(x,y) \sim \mathcal{S}} [yf_{\mathcal{A}}(x) \leq \theta] + O \left(\frac{\ln |\mathcal{H}|}{\theta^2} + \sqrt{\frac{\ln |\mathcal{H}|}{\theta^2} \Pr_{(x,y) \sim \mathcal{S}} [yf_{\mathcal{A}}(x) \leq \theta]} \right)$$

Margin-Based *Lower* Bounds

- Formally, $\forall N, \theta, \tau$ There exist a set \mathcal{X} and a hypothesis set \mathcal{H} such that for every large enough m there exists an algorithm \mathcal{A} that optimizes m and there exists a distribution \mathcal{D} for which

Assuming this is at most τ .

$$\Pr_{(x,y) \sim \mathcal{D}} [yf_{\mathcal{A}}(x) \leq 0] \geq \Pr_{(x,y) \sim \mathcal{S}} [yf_{\mathcal{A}}(x) \leq \theta] + O \left(\frac{\ln |\mathcal{H}|}{\theta^2} + \sqrt{\frac{\ln |\mathcal{H}|}{\theta^2} \Pr_{(x,y) \sim \mathcal{S}} [yf_{\mathcal{A}}(x) \leq \theta]} \right)$$

Margin-Based *Lower* Bounds

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Summary

- We show margin-based generalization lower bounds which almost match the best known upper bounds.
- These bounds essentially complete the theory of generalization bounds based on margins alone.
- Open Question : Are there parameters other than margin that can be used to better explain the practical properties of voting classifiers?