Theoretical Explanation of Boosting Algorithms

Liwei Wang

Peking University, China

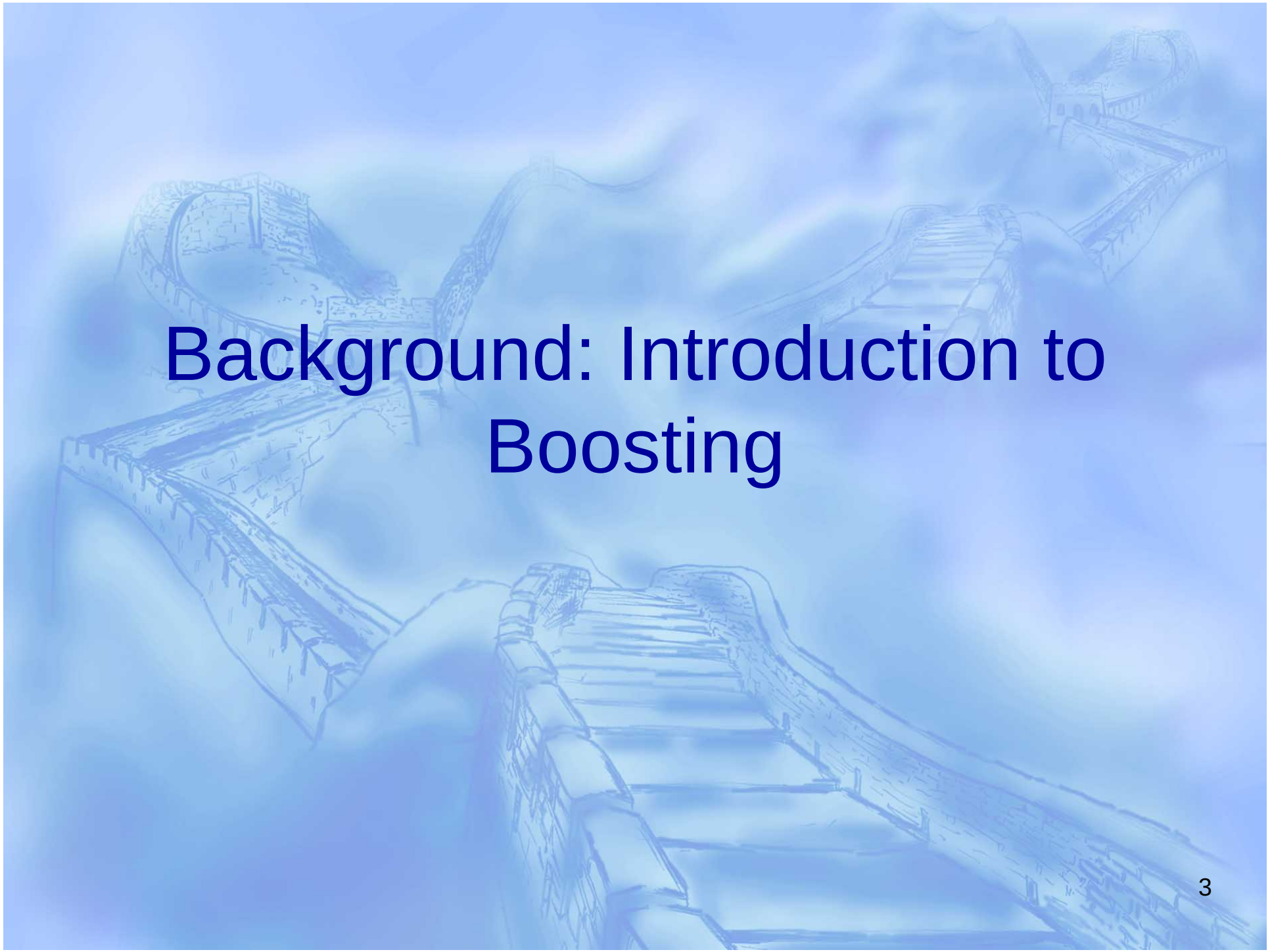
Joint work with

Masashi Sugiyama, Cheng Yang,

Zhi-Hua Zhou, and Jufu Feng

Outline

- Background: introduction to Boosting.
- Margin explanation and Breiman's doubt.
- Main result:
  - Equilibrium Margin (EMargin) bound.
- Experimental results.
- Summary and future work.



Background: Introduction to Boosting

Background

- Learning and Classification:
  - Training examples

    $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ $\quad x_i \in X, \quad y_i \in Y$

    i.i.d. from an underlying joint distribution P

  - Classifier: $C : X \rightarrow Y$

  - Generalization Error: $P(C(x) \neq y)$

Background

- Performance of Boosting:
  - AdaBoost + Decision trees + Calibration = the best classification algorithm (Caruana, 2006).
  - “Boosting is the best off-the-shelf classifier in the world” (Breiman, 1998)

- The Boosting algorithm

Input: $S = (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
where $x_i \in X$, $y_i \in \{-1, 1\}$.
Initialization: $D_1(i) = 1/n$.
for $t = 1$ **to** T **do**

1. Train base learner using distribution D_t.
2. Get base classifier $h_t : X \to \{-1, 1\}$.
3. Choose α_t.
4. 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 chosen so that D_{t+1} will be a distribution.

end
Output: The final Classifier

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

Background

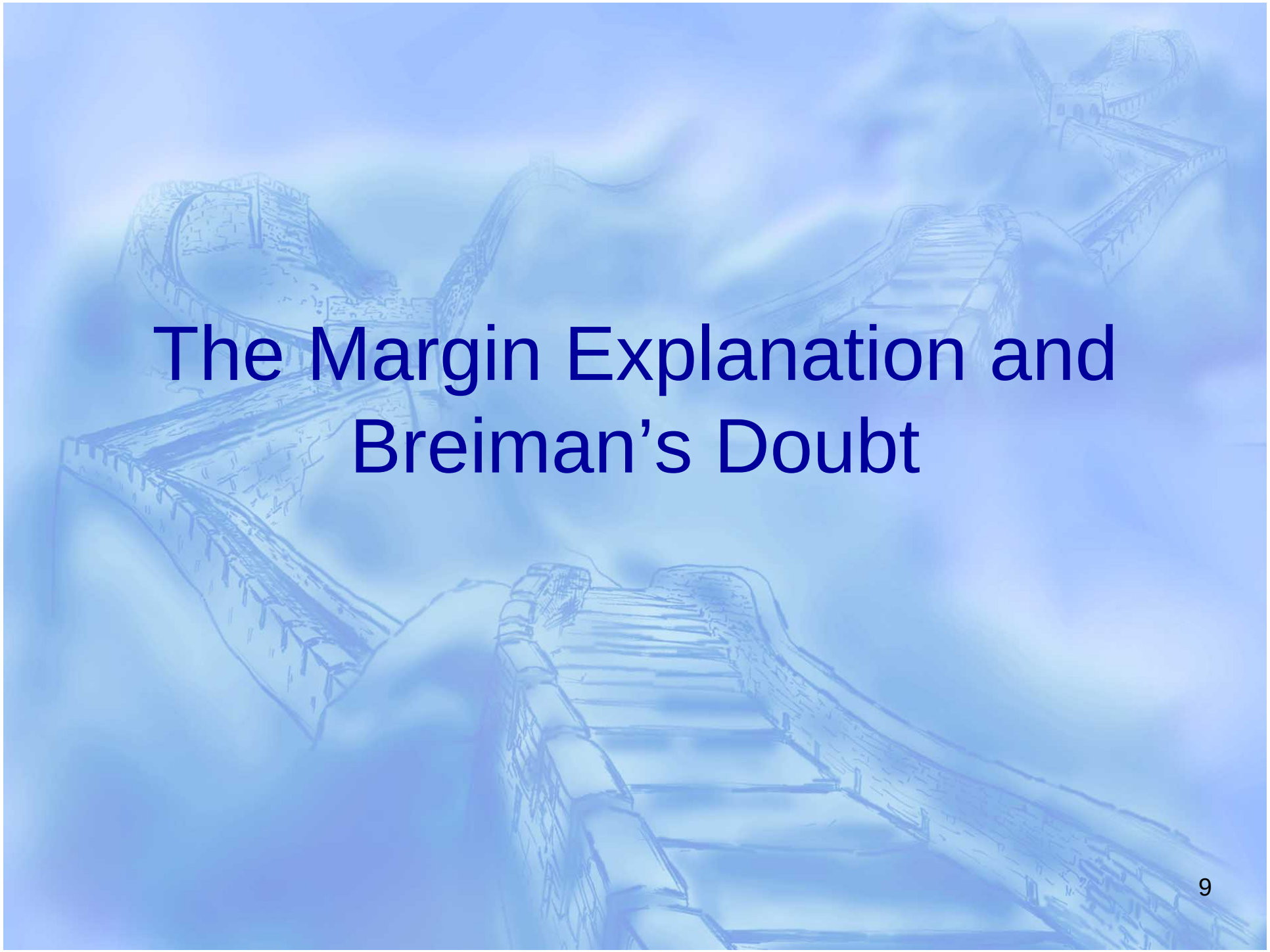
- Empirical observation:
  - AdaBoost often resists to overfitting:
    - The test error of the combined classifier usually keeps decreasing as its size becomes very large, and even after the training error is zero, which seems contradicts the Occam's razor!

- What does AdaBoost Do?
  - AdaBoost minimizes the exponential loss in a coordinate decent manner:

$$\sum_{i=1}^{n} \exp\{-y_i f(x_i)\} = \sum_{i=1}^{n} \exp\left\{-y_i \sum_{t=1}^{T} \alpha_t h_t(x_i)\right\}$$

  - If at round t, the base classifier has error rate ε_t with respect to the distribution D_t, then the exponential loss can be bounded by:

$$\sum_{i=1}^{n} \exp\{-y_i f(x_i)\} \le \prod_{t=1}^{T} \sqrt{1-(1-2\varepsilon_t)^2}.$$


The Margin Explanation and
Breiman's Doubt

Theoretical Explanation

- A complete theoretical explanation (understanding) should answer two questions:
  - Why AdaBoost often has good performance?
  - Why AdaBoost is often (though not always) immune to overfitting?

The Concept of Margin

- Margins in Boosting:
  - The combined (voting) classifier produced by the ensemble learning algorithms could be written as:

$$f(x) = \sum \alpha_i h_i(x), \qquad \sum \alpha_i = 1, \qquad \alpha_i \geq 0.$$

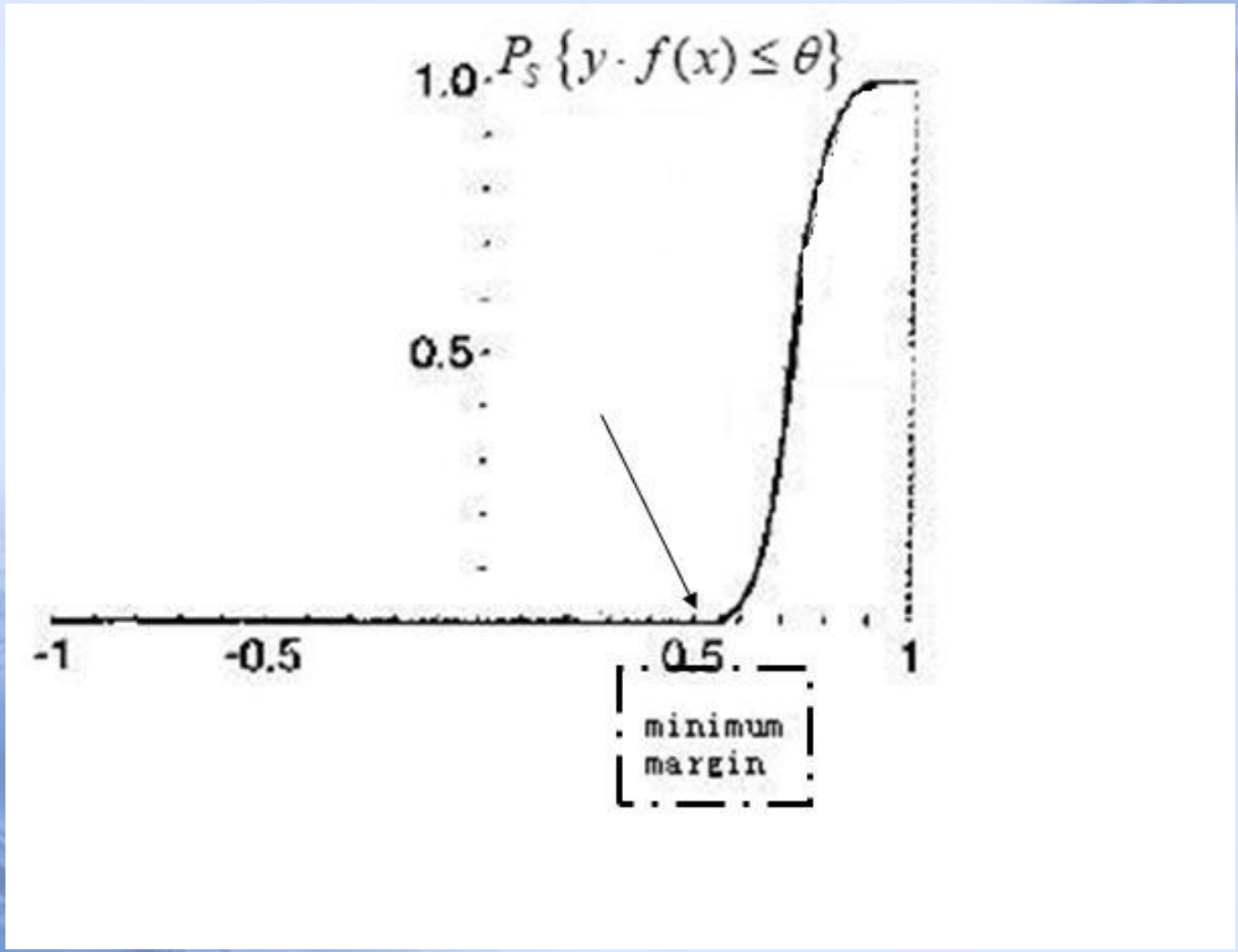
The Concept of Margin

- For binary classification, $y \in \{-1,+1\}$. The quantity $yf(x)$ is called the **margin** of the example (x, y) with respect to the classifier f.

- Margin is a confidence measure (like in SVM).

- The **minimum margin** is the smallest margin over the set of training examples.

- Margin distribution:



Margin Theory

- Margin theory is essentially upper bounds on the generalization error of the voting classifier, in terms of various **margin** notions.

The Margin Distribution Bound

- Theorem 1 (Schapire et al. 1998):
  - For any $\delta > 0$, with probability at least $1-\delta$ over the random choice of the training set S of n examples, every voting classifier satisfies the following bound:

$$P_D\left(yf(x) \le 0\right) \le \inf_{\theta \in (0,1]} \left[P_S\left(yf(x) \le \theta\right) + O\left(\frac{1}{\sqrt{n}} \left(\frac{\log n \log |H|}{\theta^2} + \log \frac{1}{\delta} \right)^{1/2} \right) \right]$$

where H is the set which the base classifiers are chosen from.

Margin Explanation

- Schapire et al. also demonstrated theoretically and empirically that AdaBoost can generate good margin distribution.
- The margin distribution keeps improving even after the training error is zero. This accounts for AdaBoost's resistance to overfitting.

- Breiman's doubt and the Arc-gv algorithm:
  - Arc-gv provably generate the largest possible minimum margin among all boosting type algorithms.

Input: $S = (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
where $x_i \in X$, $y_i \in \{-1, 1\}$.
Initialization: $D_1(i) = 1/n$.
for $t = 1$ **to** T **do**

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where Z_t is a normalization factor chosen so that D_{t+1} will be a distribution.

end
Output: The final Classifier

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

Breiman's Doubt

- The minimum margin bound (Breiman1999):

$$\forall_{\delta} \;\; P_D\left(yf(x) \le 0\right) \le R\left(\log 2n + \log\frac{1}{R} + 1\right) + \frac{1}{n}\log\left(\frac{|H|}{\delta}\right).$$

where

$$R = \frac{32\log 2\,|H|}{n\theta_0^2}$$

and θ_0 is the minimum margin.

Breiman's Doubt

- Breiman's argument:
  - The minimum margin bound is sharper than the margin distribution bound.

$$O\left(\frac{\log n}{n}\right) \text{ vs. } O\left(\sqrt{\frac{\log n}{n}}\right)$$

If the bound of Schapire et al. implies that the margin distribution is the key to the generalization error, his bound implies more stronly that the minimum margin governs the generalization error.

Breiman's Doubt

- Breiman conducted experiments, and found that arc-gv performs **consistently worse** than AdaBoost although it always generates larger minimum margins!
- Arc-gv even generates uniformly better margin distribution than AdaBoost.
- Breiman concluded that neither the margin distribution nor the minimum margin is the right explanation!

Recent Discovery

- An important discovery (Reyzin and Schapire 2006):
  - In the margin bounds, the generalization error depends not only on the margin, but also the complexity of the set of base classifiers.

$$P_D\left(yf(x)\le 0\right)\le \inf_{\theta\in(0,1]}\left[P_S\left(yf(x)\le\theta\right)+O\left(\frac{1}{\sqrt{n}}\left(\frac{\log n\log|H|}{\theta^2}+\log\frac{1}{\delta}\right)^{1/2}\right)\right]$$

  - To study how margin affects the generalization, one has to keep other factors fixed.

Recent Discovery

- Breiman's experiment:
  - Base classifiers: Using decision trees of a fixed number of leaves.
- Reyzin and Schapire's discovery:
  - Trees generated by arc-gv are much deeper than those generated by AdaBoost!
  - Deeper trees are more complex even though the number of leaves are the same!
  - Breiman's experiment is not a fair comparison.

Recent Discovery

- A fair comparison:
  - Base classifier: decision stump.
  - Results:
    - AdaBoost has better performance than arc-gv.
    - Arc-gv has larger minimum margins than AdaBoost.
    - The margin distribution generated by AdaBoost is “better” than arc-gv.

Two Problems Left

- Has Breiman's doubt been fully answered?
  - Arc-gv generates larger minimum margin yet has worse performance. Contradict to the (sharper) minimum margin bound!
  - What does it mean a "better" margin distribution?
  - Average margin?
    - Among all the voting classifiers the one that has the minimum average margin is a single base classifier that has the smallest training error.

The EMargin Explanation

- Goal of this work:
  - Give Breiman's doubt a complete answer by solving these two problems

- Main results of this work:
  - A bound for the generalization error of voting classifiers in terms of a new margin notion——Equilibrium Margin (Emargin). This bound is uniformly sharper than the minimum margin bound.
  - We show that a large Emargin implies a smaller generalization error.

- Bernoulli Relative Entropy:

$$D(q \| p) = q \log \frac{q}{p} + (1-q) \log \frac{1-q}{1-p}, \qquad 0 \le p, q \le 1.$$

  - For fixed q , D is a monotone increasing function of p for $q \le p \le 1$.

- Inverse Entropy Function:

$$D^{-1}(q,u): \quad D(q \| D^{-1}(q,u)) = u. \qquad u \ge 0.$$

- Theorem: The Emargin Bound:

$$\forall_\delta \; P_D\left(yf(x) \le 0\right) \le \frac{\log|H|}{n} + \inf_{q \in \{0, \frac{1}{n}, \frac{2}{n}, \ldots, 1\}} D^{-1}\left(q, u\left[\hat{\theta}(q)\right]\right).$$

where

$$u\left[\hat{\theta}(q)\right] = \frac{1}{n}\left(\frac{8}{\hat{\theta}^2(q)}\log\left(\frac{2n^2}{\log|H|}\right)\log|H| + \log|H| + \log\frac{n}{\delta}\right).$$

and

$$\hat{\theta}(q) = \sup\left\{\theta \in \left(\sqrt{8/|H|}, 1\right] : P_S\left(yf(x) \le \theta\right) \le q\right\}.$$

- Equilibrium Margin:
  - Let q^* be the optimal q in the EMargin bound. We call

$$\theta^* = \hat{\theta}(q^*)$$

    the Equilibrium Margin (Emargin) .
  - The name equilibrium comes from the fact q^* is exactly the empirical margin error at the Emargin θ^* .
  - Emargin bound can be simply written as:

$$P_D\left(yf(x) \le 0\right) \le \frac{\log|H|}{n} + D^{-1}\left(q^*, u(\theta^*)\right).$$

- Explanation:
  - The Emargin bound has similar flavor to the margin distribution bound. The Emargin and Emargin error depend, in a complicated way on the whole margin distribution.
  - The minimum margin is a special case when the optimal q^* is zero.

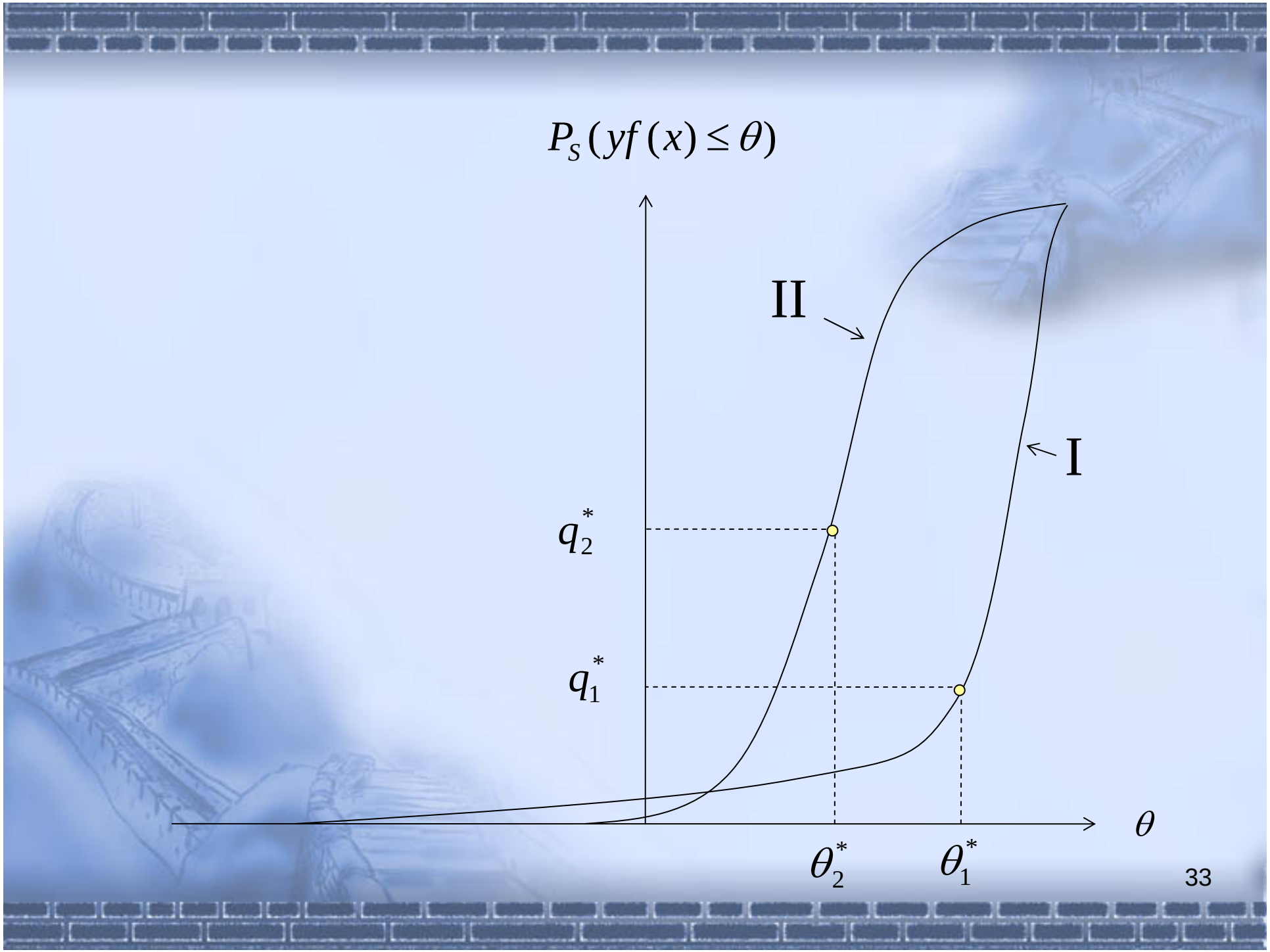
EMargin vs. Minimum Margin

- Theorem: The Emargin bound is uniformly sharper than Breiman's minimum margin bound.

- Minimum margin is not crucial for the generalization error. Arc-gv does not necessarily have better performance than AdaBoost.

- The Emargin bound implies that it is the Emargin and the Emargin error affect the generalization ability.

- Theorem: For two voting classifiers f_1, f_2, if f_1 has a larger Emargin and a smaller Emargin error than f_2, than the Emargin bound of f_1 is smaller than f_2.


$P_S(yf(x) \le \theta)$
II
I
q_2^*
q_1^*
θ
θ_2^*
θ_1^*

Further Explanation of the EMargin Bound

- By using simple upper bounds of the inverse relative entropy function, we can obtain bounds in simper forms:
  - Recover, essentially, the minimum margin bound and the margin distribution bound.
  - Derive new bound not known before.

1

$$\inf_q D^{-1}\left(q, u\left(\hat{\theta}(q)\right)\right) \le D^{-1}\left(0, u\left(\hat{\theta}(0)\right)\right) \le u\left(\hat{\theta}(0)\right).$$

$\longrightarrow$ minimum margin bound

2

$$\inf_q D^{-1}\left(q, u\left(\hat{\theta}(q)\right)\right) \le \inf_q \left(q + \left(\frac{u\left(\hat{\theta}(q)\right)}{2} \right)^{1/2} \right)$$

$\longrightarrow$ margin distribution bound

3

$$\inf_q D^{-1}\left(q, u\left(\hat{\theta}(q)\right)\right) \le \inf_{q \le Cu\left(\hat{\theta}(q)\right)} D^{-1}\left(q, u\left(\hat{\theta}(q)\right)\right)$$

$$\le \inf_{q \le Cu\left(\hat{\theta}(q)\right)} C' u\left(\hat{\theta}(q)\right).$$

$\longrightarrow$ a new $O(\frac{\log n}{n})$ bound for the nonzero error case.

Experiments

Experiments

- Setting:
  - UCI and USPS datasets.
  - Five-fold CV.
  - Binary classification.
  - Finite base classifiers.
  - Comparison of AdaBoost and Arc-gv on their EMargin, EMargin error, test error and minimum margin.

		Emargin	Emargin Error	Test Error	Minimum margin
Breast	AdaBoost	**0.313**	**0.803**	**0.052**	0.005
	arc-gv	0.281	0.909	0.057	0.008
Diabetes	AdaBoost	**0.110**	**0.748**	**0.255**	-0.064
	arc-gv	0.049	0.759	0.256	-0.017
German	AdaBoost	0.157	0.824	0.258	-0.118
	arc-gv	0.034	0.780	0.261	-0.026
Image	AdaBoost	**0.196**	**0.610**	0.023	-0.009
	arc-gv	0.195	0.705	**0.021**	-0.003
Ionosphere	AdaBoost	0.323	0.800	0.100	0.084
	arc-gv	0.131	0.577	0.106	0.061
Letter	AdaBoost	**0.078**	**0.645**	**0.174**	-0.165
	arc-gv	0.063	0.958	0.178	-0.034
Satimage	AdaBoost	**0.133**	**0.521**	**0.053**	-0.054
	arc-gv	0.133	0.956	0.057	-0.019
USPS	AdaBoost	**0.108**	**0.972**	**0.450**	-0.142
	arc-gv	0.053	0.990	0.460	-0.024
Vehicle	AdaBoost	**0.105**	**0.698**	**0.201**	-0.024
	arc-gv	0.063	0.720	0.205	-0.009
Wdbc	AdaBoost	**0.350**	**0.581**	**0.035**	-0.130
	arc-gv	0.350	0.710	**0.035**	-0.100

Experiments

- Conclusion from the experiments:
  - Usually AdaBoost has a larger EMargin and a smaller EMargin error than arc-gv. This accounts for AdaBoost's superior performances.

Summary and Future Work

Summary

- We proved an EMargin bound for voting classifiers which is uniformly sharper than the minimum margin bound.
  - It is EMargin, not minimum margin that is crucial for the generalization error of voting classifiers.
- Larger EMargin and smaller EMargin error implies smaller generalization error.

Summary

- Demonstrated that AdaBoost often generates larger EMargin and smaller EMargin error than Arc-gv.
- Gave Breiman's doubt a negative answer.

Future Work

- Can our EMargin theory explain other phenomena of Boosting algorithms observed in experiments?
  - When AdaBoost overfits, is it because a bad margin distribution?
- Can we develop an algorithm to optimize the EMargin and EMargin error? If such an algorithm exists, does it outperform AdaBoost as the theory predicts?


Thanks