Cross Validation & Ensembling

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Machine Learning

Outline

1. **Cross Validation**
   - How Many Folds?
2. **Ensemble Methods**
   - Voting
   - Bagging
   - Boosting
   - Why AdaBoost Works?

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  - Performance reporting: testing set
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  - Hyperparameter tuning: validation set
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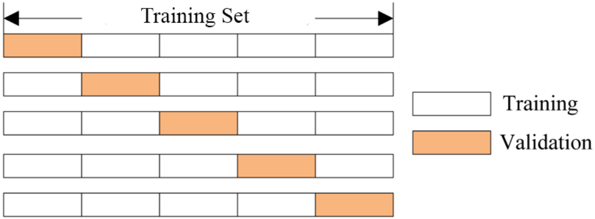
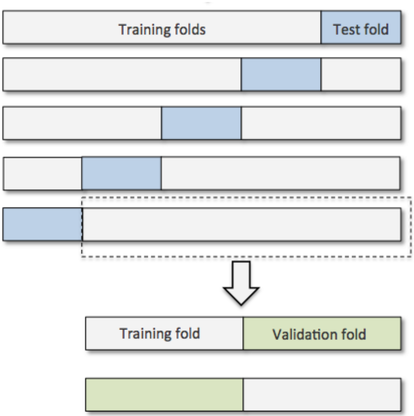
- What if we get an "unfortunate" split?
- ***K-fold cross validation***:
  1. Split the data set $\mathbb{X}$ evenly into K subsets $\mathbb{X}^{(i)}$ (called ***folds***)
  2. For $i = 1, \cdots, K$, train $f_{-N^{(i)}}$ using all data but the i-th fold ($\mathbb{X} \backslash \mathbb{X}^{(i)}$)
  3. Report the ***cross-validation error*** C_{CV} by averaging all testing errors $C[f_{-N^{(i)}}]$'s on $\mathbb{X}^{(i)}$



Nested Cross Validation

- Cross validation (CV) can be applied to ***both*** hyperparameter tuning and performance reporting



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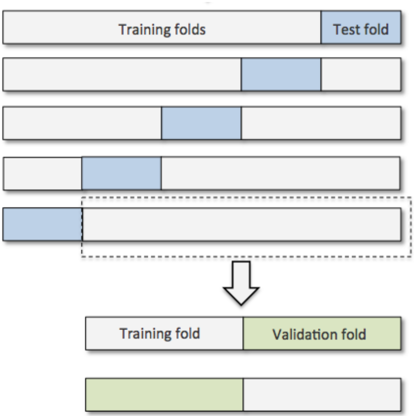

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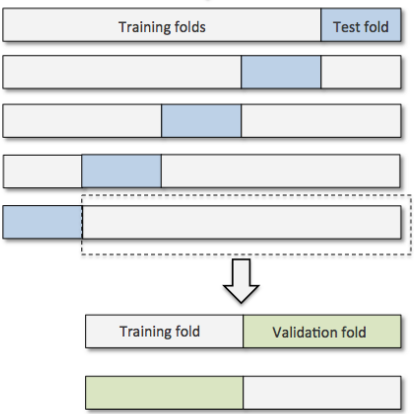

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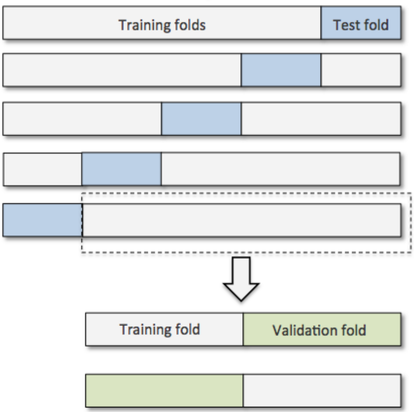

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1. Inner (2 folds): select hyperparameters giving lowest C_{CV}
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3. Outer (5 folds): report C_{CV} as test error

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- The cross-validation error C_{CV} is an average of $C[f_{-N^{(i)}}]$'s
- Regard each $C[f_{-N^{(i)}}]$ as an estimator of the expected generalization error $\mathrm{E}_{\mathbb{X}}(C[f_N])$
- C_{CV} is an estimator too, and we have

$$\mathrm{MSE}(C_{\text{CV}}) = \mathrm{E}_{\mathbb{X}}[(C_{\text{CV}} - \mathrm{E}_{\mathbb{X}}(C[f_N]))^2] = \mathrm{Var}_{\mathbb{X}}(C_{\text{CV}}) + \mathrm{bias}(C_{\text{CV}})^2$$

Point Estimation Revisited: Mean Square Error

- Let $\hat{\theta}_n$ be an estimator of quantity θ related to random variable $\mathbf{x}$ mapped from n i.i.d samples of $\mathbf{x}$
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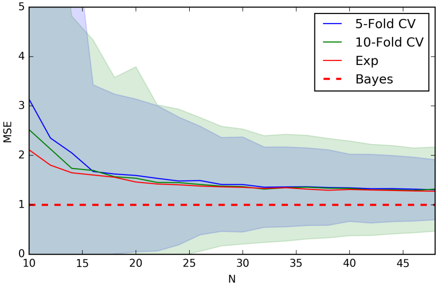
&= \mathrm{Var}_{\mathbb{X}}(\hat{\theta}_n) + \mathrm{bias}(\hat{\theta}_n)^2
\end{aligned}$$

- MSE of an unbiased estimator is its variance

Example: 5-Fold vs. 10-Fold CV

$$\mathrm{MSE}(C_{\mathrm{CV}}) = \mathrm{E}_{\mathbb{X}}[(C_{\mathrm{CV}} - \mathrm{E}_{\mathbb{X}}(C[f_N]))^2] = \mathrm{Var}_{\mathbb{X}}(C_{\mathrm{CV}}) + \mathrm{bias}(C_{\mathrm{CV}})^2$$



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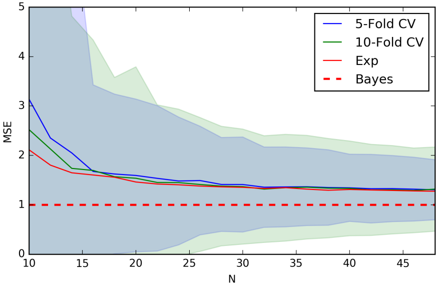

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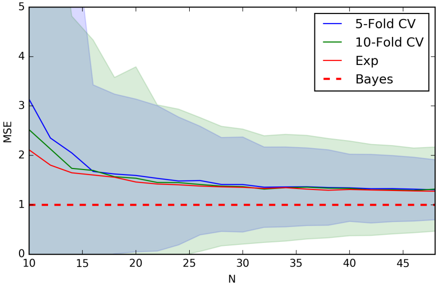

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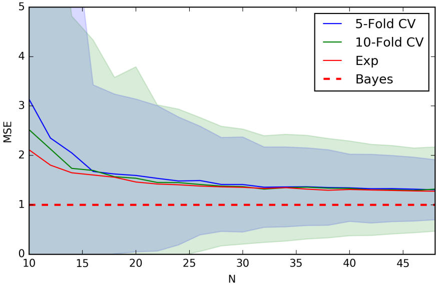

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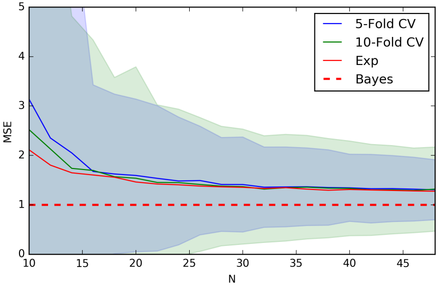

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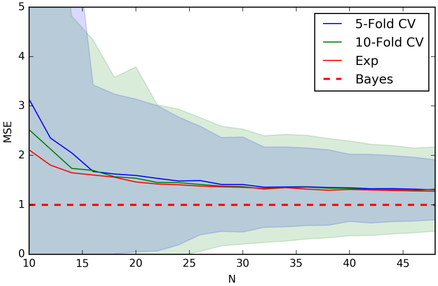

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- We can reduce $\text{bias}(C_{\text{CV}})$ and $\text{Var}(C_{\text{CV}})$ by ***learning theory***
  - Choosing the right model complexity avoiding both underfitting and overfitting
  - Collecting more training examples (N)

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- We can reduce $\text{bias}\left(C_{\text{CV}}\right)$ and $\text{Var}\left(C_{\text{CV}}\right)$ by ***learning theory***
  - Choosing the right model complexity avoiding both underfitting and overfitting
  - Collecting more training examples (N)
- Furthermore, we can reduce $\text{Var}\left(C_{\text{CV}}\right)$ by ***making*** $f_{-N^{(i)}}$ ***and*** $f_{-N^{(j)}}$ ***uncorrelated***

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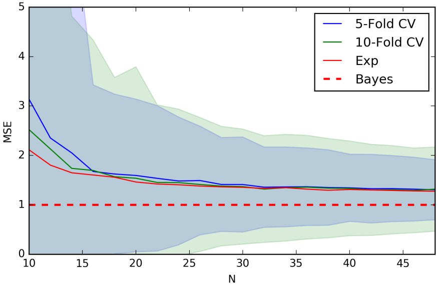

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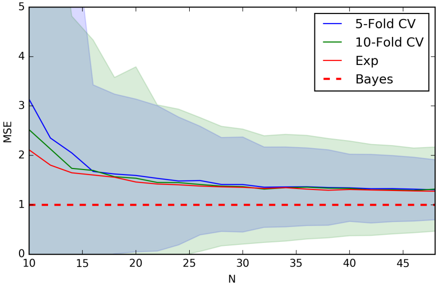
    - High $\text{Cov}\left(C[f_{-N^{(i)}}], C[f_{-N^{(j)}}]\right)$, as training sets $\mathbb{X}\backslash\mathbb{X}^{(i)}$ and $\mathbb{X}\backslash\mathbb{X}^{(j)}$ are more similar thus $C[f_{-N^{(i)}}]$ and $C[f_{-N^{(j)}}]$ are more positively correlated



How Many Folds K? IV

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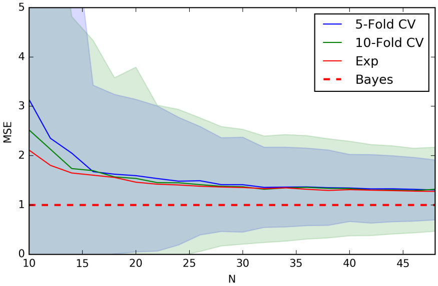
- Conversely, with a small K, the cross-validation error tends to have a high $\text{bias}\left(C[f_{-N^{(s)}}]\right)$ and $\text{Var}\left(C[f_{-N^{(s)}}]\right)$ but low $\text{Cov}\left(C[f_{-N^{(i)}}], C[f_{-N^{(j)}}]\right)$



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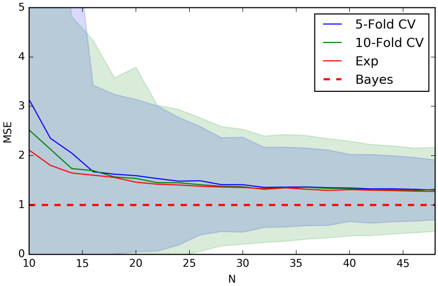
- In practice, we usually set $K = 5$ or 10



Leave-One-Out CV

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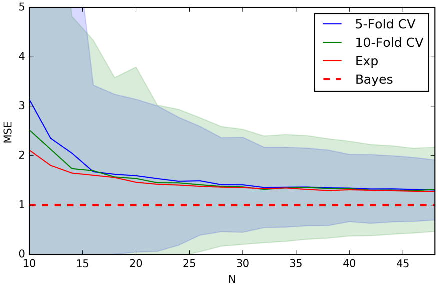

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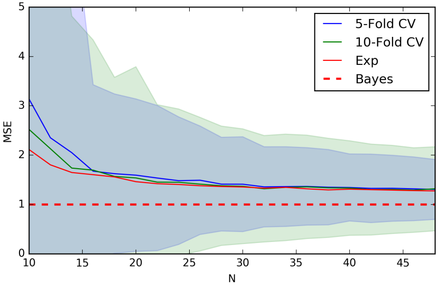
- We can choose $K = N$, which we call the ***leave-one-out CV***



Outline

1. Cross Validation
   - How Many Folds?
2. **Ensemble Methods**
   - Voting
   - Bagging
   - Boosting
   - Why AdaBoost Works?

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- How to "combine" multiple base-learners?

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Voting

- ***Voting***: linear combining the predictions of base-learners for each $\boldsymbol{x}$:

$$\tilde{y}_k = \sum_j w_j \hat{y}_k^{(j)} \text{ where } w_j \geq 0, \sum_j w_j = 1.$$

- If all learners are given equal weight $w_j = 1/L$, we have the ***plurality vote*** (multi-class version of majority vote)

Voting Rule	Formular
Sum	$\tilde{y}_k = \frac{1}{L}\sum_{j=1}^{L} \hat{y}_k^{(j)}$
Weighted sum	$\tilde{y}_k = \sum_j w_j \hat{y}_k^{(j)}, w_j \geq 0, \sum_j w_j = 1$
Median	$\tilde{y}_k = \text{median}_j \hat{y}_k^{(j)}$
Minimum	$\tilde{y}_k = \min_j \hat{y}_k^{(j)}$
Maximum	$\tilde{y}_k = \max_j \hat{y}_k^{(j)}$
Product	$\tilde{y}_k = \prod_j \hat{y}_k^{(j)}$

Why Voting Works? I

Why Voting Works? I

- Assume that each $\hat{y}^{(j)}$ has the expected value $\mathrm{E}_{\mathbb{X}}\left(\hat{y}^{(j)}\,|\,\boldsymbol{x}\right)$ and variance $\mathrm{Var}_{\mathbb{X}}\left(\hat{y}^{(j)}\,|\,\boldsymbol{x}\right)$
- When $w_j = 1/L$, we have:

$$\mathrm{E}_{\mathbb{X}}\left(\tilde{y}\,|\,\boldsymbol{x}\right) = \mathrm{E}\left(\sum_j \frac{1}{L}\hat{y}^{(j)}\,|\,\boldsymbol{x}\right) = \frac{1}{L}\sum_j \mathrm{E}\left(\hat{y}^{(j)}\,|\,\boldsymbol{x}\right) = \mathrm{E}\left(\hat{y}^{(j)}\,|\,\boldsymbol{x}\right)$$

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- The expected value doesn't change, so the bias doesn't change

Why Voting Works? II

$$\mathrm{Var}_{\mathbb{X}}(\tilde{y}\,|\,\boldsymbol{x}) = \frac{1}{L}\mathrm{Var}\left(\hat{y}^{(j)}\,|\,\boldsymbol{x}\right) + \frac{2}{L^2}\sum_{i,j,i<j}\mathrm{Cov}\left(\hat{y}^{(i)},\hat{y}^{(j)}\,|\,\boldsymbol{x}\right)$$

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- If $\hat{y}^{(i)}$ and $\hat{y}^{(j)}$ are uncorrelated, the variance can be reduced
- Unfortunately, $\hat{y}^{(j)}$'s may ***not*** be i.i.d. in practice
- If voters are positively correlated, variance increases

Outline

Bagging

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- How?

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1. Generate L slightly different samples from a given sample is done by ***bootstrap***: given $\mathbb{X}$ of size N, we draw N points randomly from $\mathbb{X}$ ***with replacement*** to get $\mathbb{X}^{(j)}$
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2. Train a base-learner for each $\mathbb{X}^{(j)}$

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- How? Why not train the next learner on the mistakes of the previous learners
- For simplicity, let's consider the binary classification here: $d^{(j)}(\boldsymbol{x}) \in \{1, -1\}$
- The original boosting algorithm combines three ***weak learners*** to generate a ***strong learner***
  - A week learner has error probability less than $1/2$ (better than random guessing)
  - A strong learner has arbitrarily small error probability

Original Boosting Algorithm

- Training

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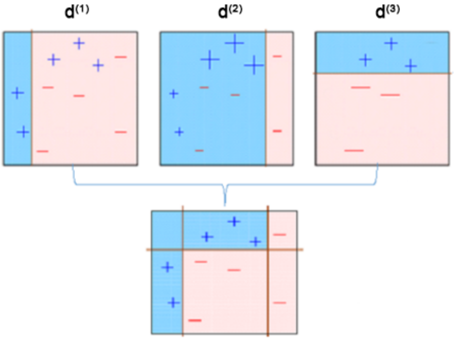
2. Otherwise the output of $d^{(3)}$ is taken

Example

- Assuming $\mathbb{X}^{(1)}$, $\mathbb{X}^{(2)}$, and $\mathbb{X}^{(3)}$ are the same:



- Disadvantage: requires a large training set to afford the three-way split

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- How to make some points "larger?"
- Modify the probabilities of drawing the instances as a function of error
- Notation:
- $\mathrm{Pr}^{(i,j)}$: probability that an example $(\boldsymbol{x}^{(i)}, y^{(i)})$ is drawn to train the jth base-learner $d^{(j)}$
- $\varepsilon^{(j)} = \sum_i \mathrm{Pr}^{(i,j)} 1(y^{(i)} \neq d^{(j)}(\boldsymbol{x}^{(i)}))$: error rate of $d^{(j)}$ on its training set

Algorithm

- Training

1. Initialize $\Pr^{(i,1)} = \frac{1}{N}$ for all i
2. Start from $j = 1$:
    1. Randomly draw N examples from $\mathbb{X}$ with probabilities $\Pr^{(i,j)}$ and use them to train $d^{(j)}$

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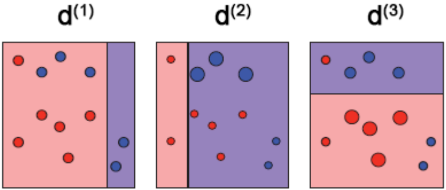
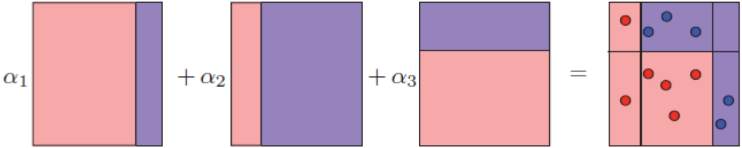
- Testing

1. Given $\boldsymbol{x}$, calculate $\hat{y}^{(j)}$ for all j
2. Make final prediction $\tilde{y}$ by voting: $\tilde{y} = \sum_j \alpha_j d^{(j)}(\boldsymbol{x})$

Example





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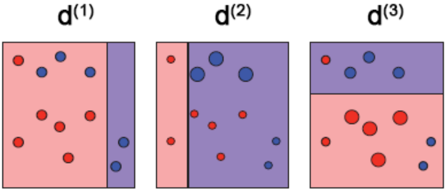

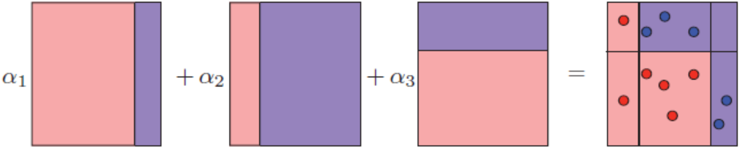

- $d^{(j+1)}$ complements $d^{(j)}$ and $d^{(j-1)}$ by focusing on predictions they disagree
- Voting weights ($\alpha_j = \frac{1}{2}\log\left(\frac{1-\varepsilon^{(j)}}{\varepsilon^{(j)}}\right)$) in predictions are proportional to the base-learner's accuracy

Outline

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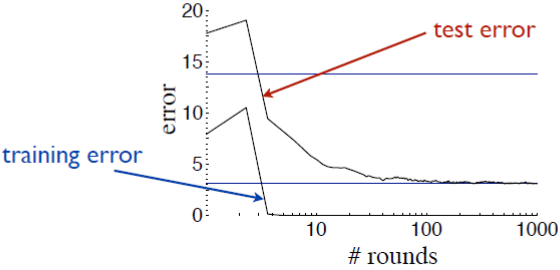

C4.5 decision trees (Schapire et al., 1998).

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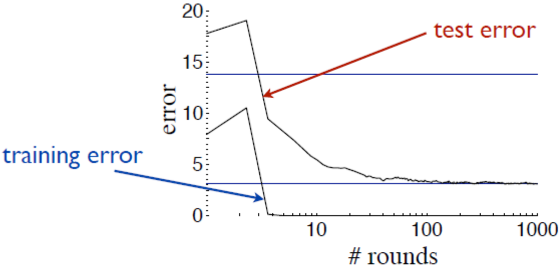
- AdaBoost ***increases margin*** [1, 2]



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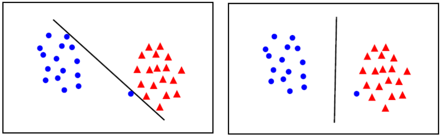
Margin as Confidence of Predictions

- Recall in SVC, a larger margin improves generalizability



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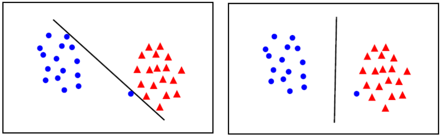

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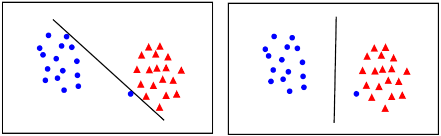


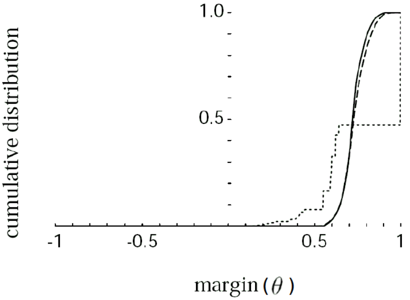
- We can define the margin for AdaBoost similarly
- In binary classification, define ***margin*** of a prediction of an example $(\boldsymbol{x}^{(i)}, y^{(i)}) \in \mathbb{X}$ as:

$$margin(\boldsymbol{x}^{(i)}, y^{(i)}) = y^{(i)} f(\boldsymbol{x}^{(i)}) = \sum_{j: y^{(i)} = d^{(j)}(\boldsymbol{x}^{(i)})} \alpha_j - \sum_{j: y^{(i)} \neq d^{(j)}(\boldsymbol{x}^{(i)})} \alpha_j$$

Margin Distribution

- Margin distribution over θ:

$$\Pr_{\mathbb{X}}(y^{(i)}f(\boldsymbol{x}^{(i)}) \leq \theta) \approx \frac{|(\boldsymbol{x}^{(i)}, y^{(i)}) : y^{(i)}f(\boldsymbol{x}^{(i)}) \leq \theta|}{|\mathbb{X}|}$$



LEGEND: (small dash, large dash, solid) lines equal (5, 100, 1000) rounds of boosting

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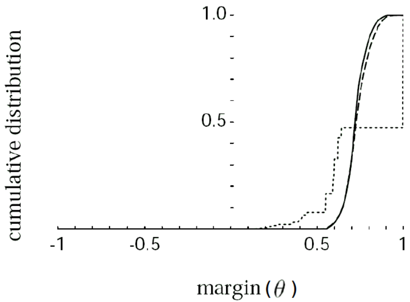

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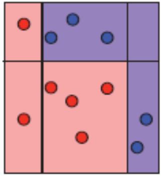
- A complementary learner:
- Clarifies low confidence areas
- Increases margin of points in these areas



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