Cross Validation & Ensembling

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Machine Learning

Outline

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

Cross Validation

- So far, we use the ***hold out*** method for:
  - Hyperparameter tuning: validation set
  - Performance reporting: testing set
- What if we get an "unfortunate" split?

Cross Validation

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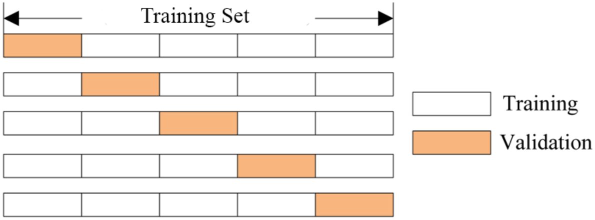
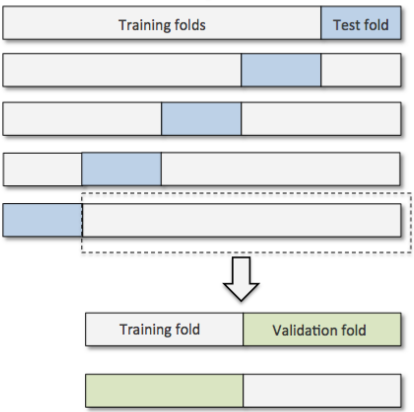
  - Hyperparameter tuning: validation set
  - Performance reporting: testing set
- What if we get an "unfortunate" split?
- ***K-fold cross validation***:
  1. Split the data set $\mathbb{X}$ evenly into K subsets $\mathbb{X}^{(i)}$ (called ***folds***)
  2. For $i = 1, \cdots, K$, train $f_{-N^{(i)}}$ 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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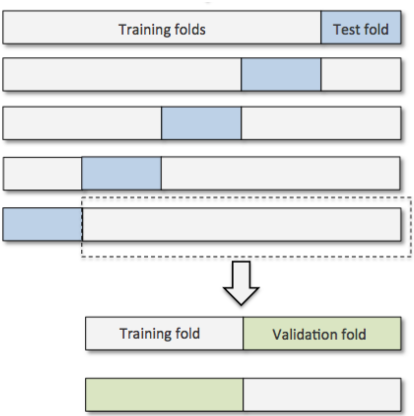

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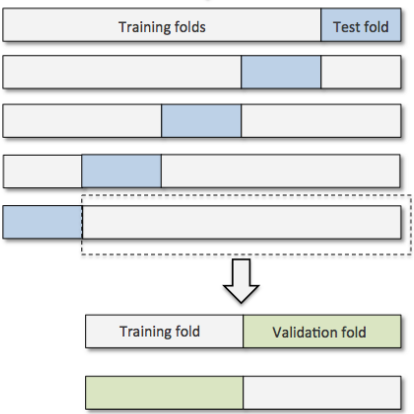

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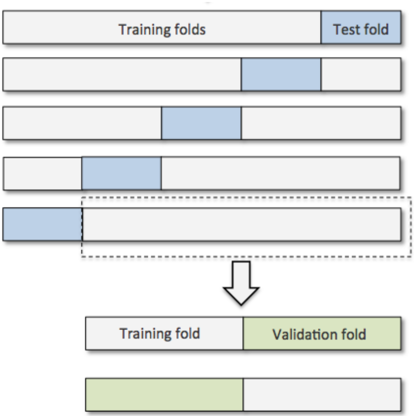

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1. Inner (2 folds): select hyperparameters giving lowest C_{CV}
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3. Outer (5 folds): report C_{CV} as test error

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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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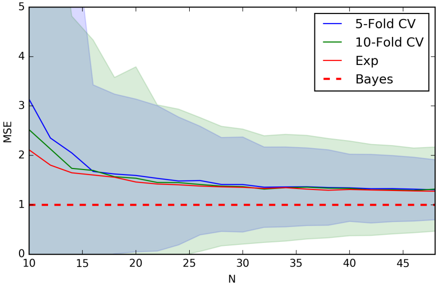
&= \mathrm{Var}_{\mathbb{X}}(\hat{\theta}_n) + \mathrm{bias}(\hat{\theta}_n)^2
\end{aligned}$$

- MSE of an unbiased estimator is its variance

我們喜歡unbiased的θ
因為它的MSE就是variance

Example: 5-Fold vs. 10-Fold CV

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



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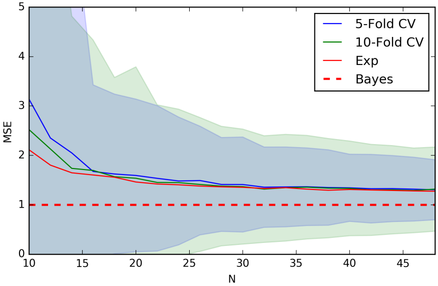
- Consider polynomial regression where $\mathrm{P}(\mathrm{y}|\mathrm{x}) = \sin(x) + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2)$



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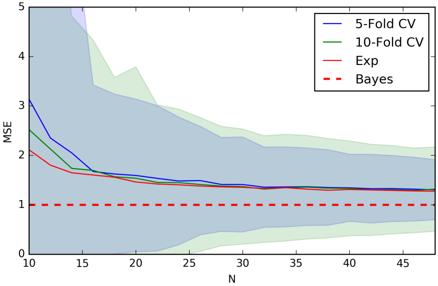

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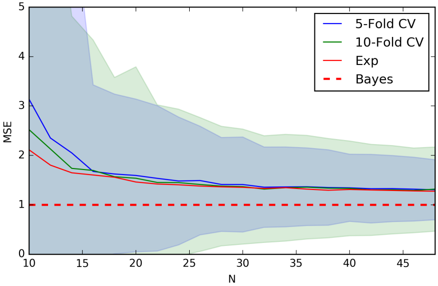

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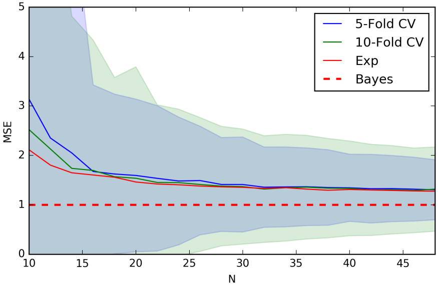

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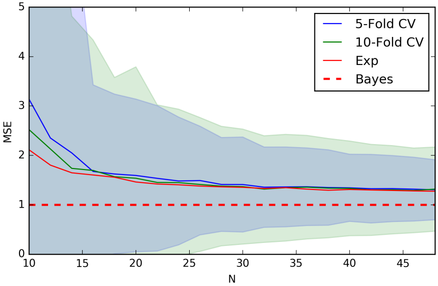
- $\mathrm{Var}_{\mathbb{X}}(C_{\mathsf{CV}})$: shaded areas

fold 較少 bias 較大 但 var會較小



Decomposing Bias and Variance

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trade off

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

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$$\text{Var}\left(C_{\text{CV}}\right) = \frac{1}{K}\text{Var}\left(C[f_{-N^{(s)}}]\right) + \frac{2}{K^2}\sum_{i,j,j>i}\text{Cov}\left(C[f_{-N^{(i)}}], C[f_{-N^{(j)}}]\right), \forall s$$

- 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***

How Many Folds K? III

$$\text{bias}\left(C_{\text{CV}}\right) = \text{bias}\left(C[f_{-N^{(s)}}]\right), \forall s$$
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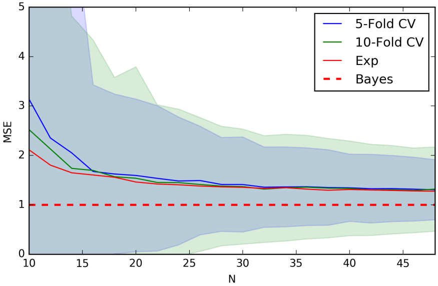

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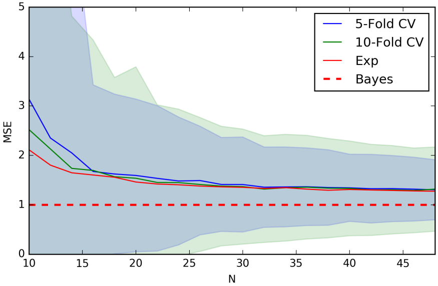
  - High $\text{Cov}\left(C[f_{-N^{(i)}}],C[f_{-N^{(j)}}]\right)$, as training sets $\mathbb{X}\backslash\mathbb{X}^{(i)}$ and $\mathbb{X}\backslash\mathbb{X}^{(j)}$ are more similar thus $C[f_{-N^{(i)}}]$ and $C[f_{-N^{(j)}}]$ are more positively correlated



K 越大　data set會被切越細
每次都99% train 1%validation
那每一次拿來train的資料都會很相似
Cov(i,j)會高

How Many Folds K? IV

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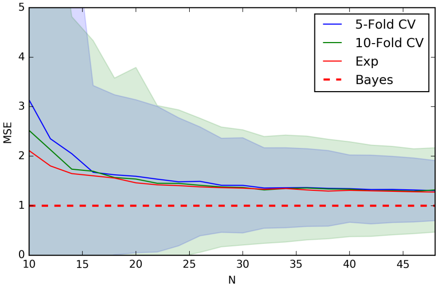
- Conversely, with a small K, the cross-validation error tends to have a high bias $\left(C[f_{-N^{(s)}}]\right)$ and Var $\left(C[f_{-N^{(s)}}]\right)$ but low Cov $\left(C[f_{-N^{(i)}}], C[f_{-N^{(j)}}]\right)$



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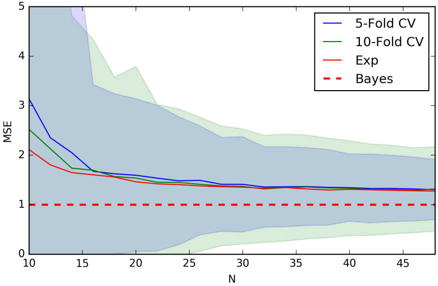
- In practice, we usually set $K=5$ or 10

data set很大的話選3 or 5　　data set 普通的話 選10 可以降低一些var的影響



Leave-One-Out CV

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- For very small dataset:
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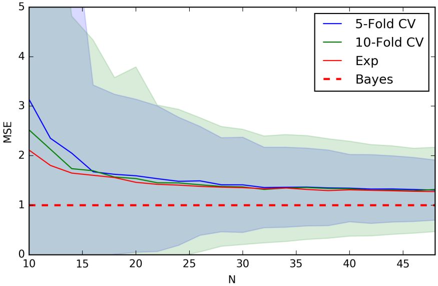

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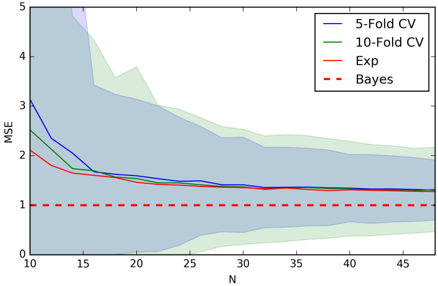
  - Not $\text{Cov}\left(C[f_{-\mathbb{N}^{(i)}}], C[f_{-\mathbb{N}^{(j)}}]\right)$
- We can choose $K = N$, which we call the ***leave-one-out CV***



Outline

Ensemble Methods

- ***No free lunch theorem***: there is no single ML algorithm that always outperforms the others in all domains/tasks

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- These are the goals of ***ensemble learning***
- How to "combine" multiple base-learners?

Outline

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

- ***Bagging*** (short for ***bootstrap aggregating***) is a voting method, but base-learners are made different deliberately
- How?

Bagging

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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 $\mathbb{X}^{(j)}$
    - It is possible that some instances are drawn more than once and some are not at all

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2. Train a base-learner for each $\mathbb{X}^{(j)}$

Outline

Boosting

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- In ***boosting***, we generate ***complementary*** base-learners
- 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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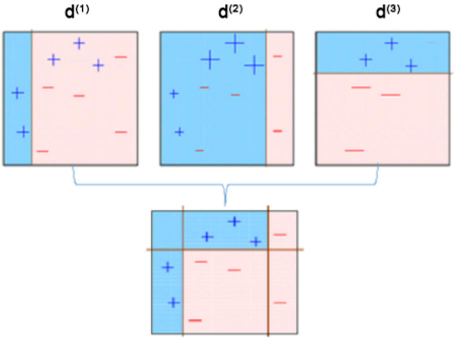
d1和d2預測的不同的那些. 丟去train d3

- Testing

1. Feed a point it to $d^{(1)}$ and $d^{(2)}$ first. If their outputs agree, use them as the final prediction
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

AdaBoost

- ***AdaBoost***: uses the same training set over and over again
- How to make some points "larger?"

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- ***AdaBoost***: uses the same training set over and over again
- 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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    2. Stop adding new base-learners if $\varepsilon^{(j)} \geq \frac{1}{2}$

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    3. Define $\alpha_j = \frac{1}{2}\log\left(\frac{1-\varepsilon^{(j)}}{\varepsilon^{(j)}}\right) > 0$ and set $\Pr^{(i,j+1)} = \Pr^{(i,j)} \cdot \exp(-\alpha_j y^{(i)} d^{(j)}(\boldsymbol{x}^{(i)}))$ for all i

預測對的話 exp(-a) = 1 / exp(a) 機率變小
預測錯的話 exp(a) 抽到的機率變大

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    4. Normalize $\Pr^{(i,j+1)}$, $\forall i$, by multiplying $\left(\sum_i \Pr^{(i,j+1)}\right)^{-1}$

再normalize讓所有機率加起來還是1

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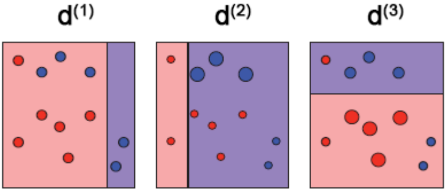
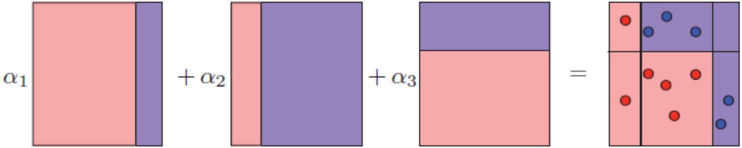
- Testing

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

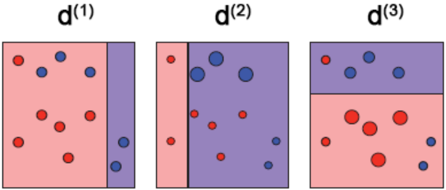
Example

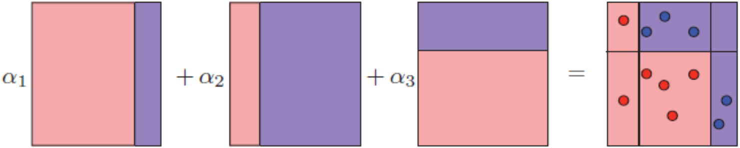




- $d^{(j+1)}$ complements $d^{(j)}$ and $d^{(j-1)}$ by focusing on predictions they disagree

Example





- $d^{(j+1)}$ 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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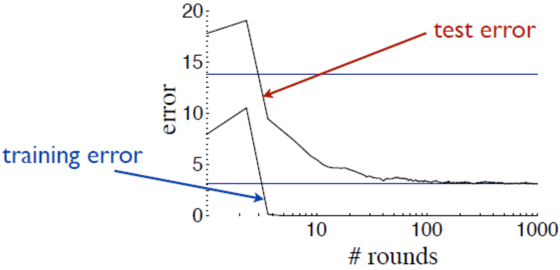

C4.5 decision trees (Schapire et al., 1998).

Why AdaBoost Works

- Why AdaBoost improves performance?
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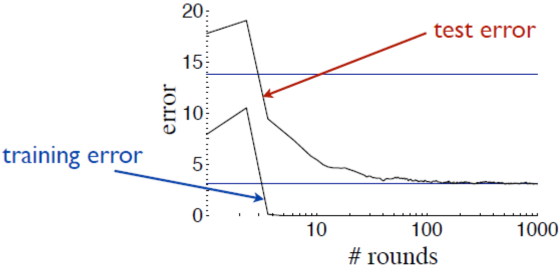
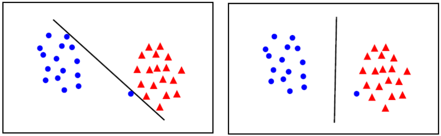
  - Empirical study: AdaBoost ***reduces overfitting*** as L grows, even when there is no training error
- AdaBoost ***increases margin*** [1, 2]



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

Margin as Confidence of Predictions

- Recall in SVC, a larger margin improves generalizability



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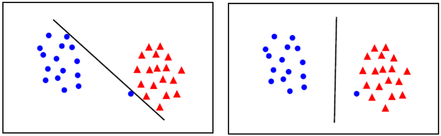

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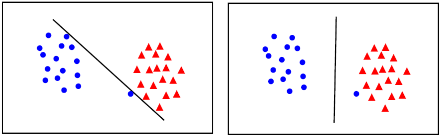


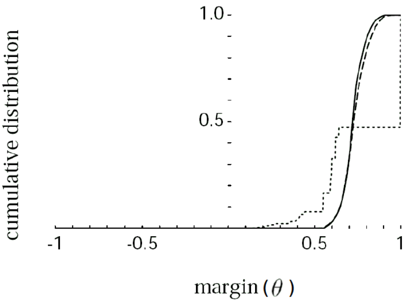
- We can define the margin for AdaBoost similarly
- In binary classification, define ***margin*** of a prediction of an example $(\boldsymbol{x}^{(i)}, y^{(i)}) \in \mathbb{X}$ as:

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

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

increase rounds 大家的margin都提高了

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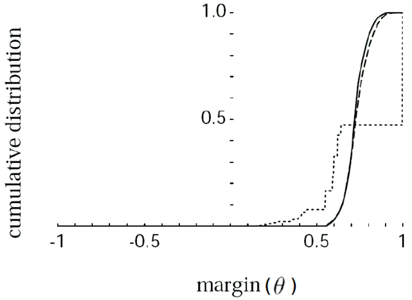

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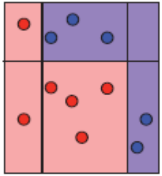
- A complementary learner:
- Clarifies low confidence areas
- Increases margin of points in these areas



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[1] Yoav Freund, Robert Schapire, and N Abe.
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[2] Liwei Wang, Masashi Sugiyama, Cheng Yang, Zhi-Hua Zhou, and Jufu Feng.
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