

*CS840a*  
*Learning and Computer Vision*  
*Prof. Olga Veksler*

Lecture 4

**Cross Validation, Bagging  
and Boosting**

Cross Validation slides are from Andrew Moore  
(CMU)

Some slides are due to Robin Dhamankar  
Vandi Verma & Sebastian Thrun

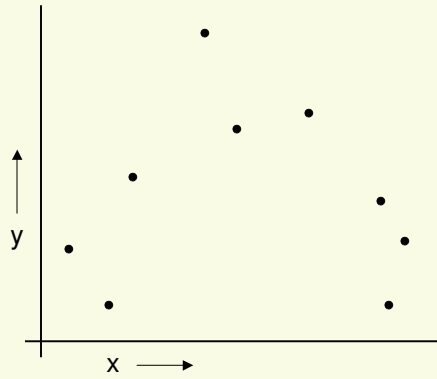
*Today*

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- New Machine Learning Topics:
  - 1) Performance evaluation methods
    - cross-validation
  - 2) Ensemble Learning
    - Bagging
    - Boosting
- Next time **two** papers:
  - “Rapid Object Detection using a Boosted Cascade of Simple Features” by P. Viola and M. Jones from CVPR2001
  - “Detecting Pedestrians Using Patterns of Motion and Appearance” by P. Viola, M.J.Jones, D. Snow

## A Regression Problem

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$$y = f(x) + \text{noise}$$

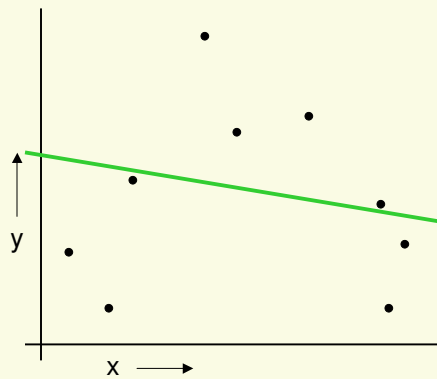
Can we learn  $f$  from this data?

Let's consider three methods...

from Andrew Moore (CMU)

## Linear Regression

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from Andrew Moore (CMU)

## Linear Regression

Univariate Linear regression with a constant term:

X	Y
3	7
1	3
⋮	⋮



$$\mathbf{X} = \begin{bmatrix} 3 \\ 1 \\ \vdots \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 7 \\ 3 \\ \vdots \end{bmatrix}$$

$\mathbf{x}_1 = (3) \dots$        $y_1 = 7 \dots$

from Andrew Moore (CMU)

## Linear Regression

Univariate Linear regression with a constant term:

X	Y
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$$\mathbf{X} = \begin{bmatrix} 3 \\ 1 \\ \vdots \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 7 \\ 3 \\ \vdots \end{bmatrix}$$

$y_1 = 7 \dots$

$$\mathbf{Z} = \begin{bmatrix} 1 & 3 \\ 1 & 1 \\ \vdots & \vdots \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 7 \\ 3 \\ \vdots \end{bmatrix}$$

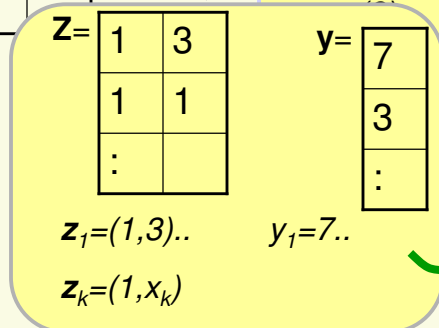
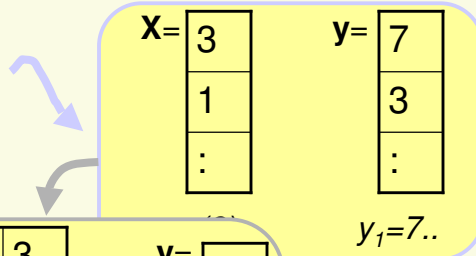
$\mathbf{z}_1 = (1, 3) \dots$        $y_1 = 7 \dots$   
 $\mathbf{z}_k = (1, x_k)$

from Andrew Moore (CMU)

## Linear Regression

Univariate Linear regression with a constant term:

X	Y
3	7
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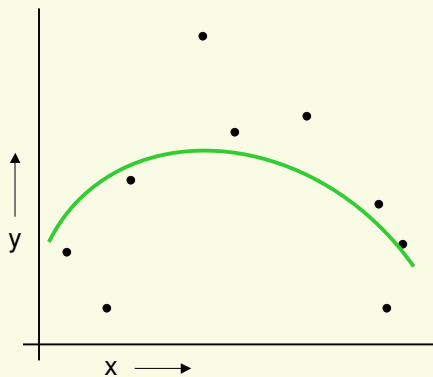


$$\beta = (Z^T Z)^{-1} (Z^T y)$$

$$y^{est} = \beta_0 + \beta_1 x$$

from Andrew Moore (CMU)

## Quadratic Regression



from Andrew Moore (CMU)

## Quadratic Regression

X	Y
3	7
1	3
⋮	⋮

$x = \begin{bmatrix} 3 \\ 1 \\ \vdots \end{bmatrix}$

$y = \begin{bmatrix} 7 \\ 3 \\ \vdots \end{bmatrix}$

$y_i = 7..$

$z = \begin{bmatrix} 1 & 3 & 9 \\ 1 & 1 & 1 \\ \vdots & \vdots & \vdots \end{bmatrix}$

$y = \begin{bmatrix} 7 \\ 3 \\ \vdots \end{bmatrix}$

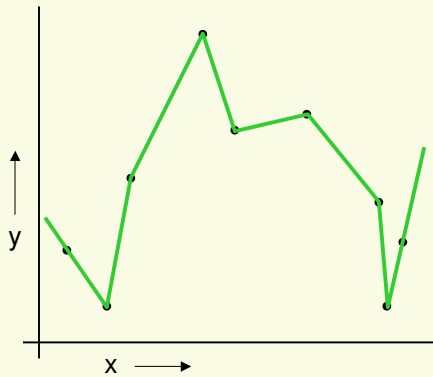
$z = (1, x, x^2)$

$$\beta = (Z^T Z)^{-1} (Z^T y)$$

$$y^{est} = \beta_0 + \beta_1 x + \beta_2 x^2$$

from Andrew Moore (CMU)

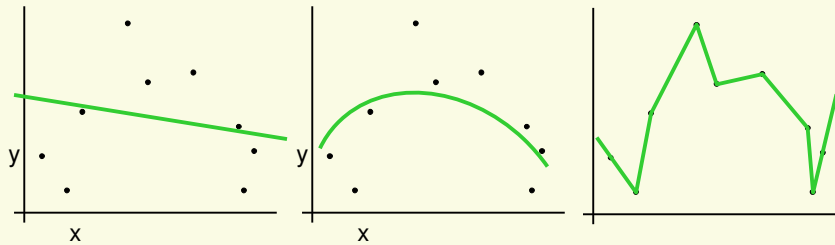
## Join-the-dots



Also known as **piecewise linear nonparametric regression** if that makes you feel better

from Andrew Moore (CMU)

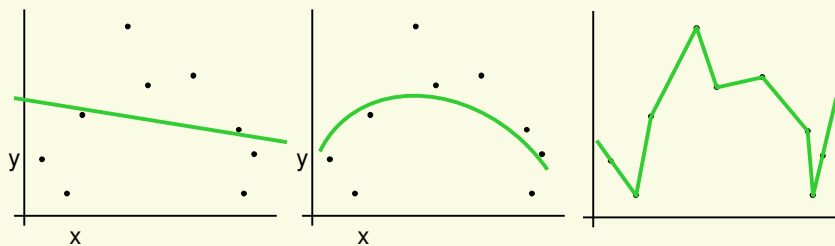
## Which is best?



Why not choose the method with the best fit to the data?

from Andrew Moore (CMU)

## What do we really want?

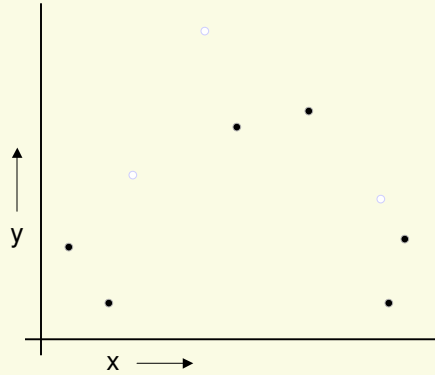


Why not choose the method with the best fit to the data?

“How well are you going to predict future data drawn from the same distribution?”

from Andrew Moore (CMU)

## The test set method

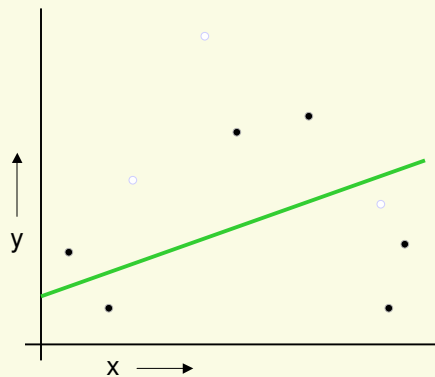


1. Randomly choose 30% of the data to be in a test set

2. The remainder is a training set

from Andrew Moore (CMU)

## The test set method



1. Randomly choose 30% of the data to be in a test set

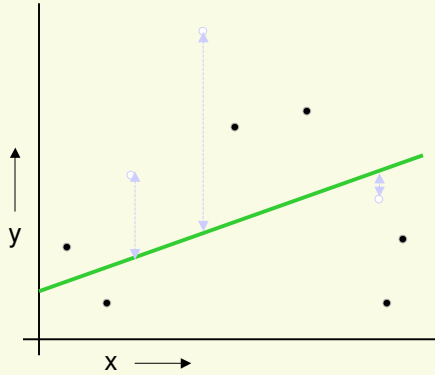
2. The remainder is a training set

3. Perform your regression on the training set

(Linear regression example)

from Andrew Moore (CMU)

## The test set method



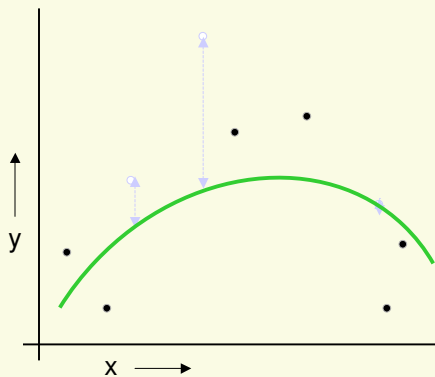
(Linear regression example)

Mean Squared Error = 2.4

1. Randomly choose 30% of the data to be in a test set
2. The remainder is a training set
3. Perform your regression on the training set
4. Estimate your future performance with the test set

from Andrew Moore (CMU)

## The test set method



(Quadratic regression example)

Mean Squared Error = 0.9

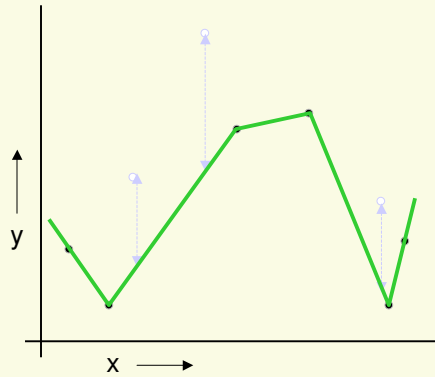
1. Randomly choose 30% of the data to be in a test set
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from Andrew Moore (CMU)



## The test set method

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1. Randomly choose 30% of the data to be in a test set
2. The remainder is a training set
3. Perform your regression on the training set
4. Estimate your future performance with the test set

from Andrew Moore (CMU)

## The test set method

---

- Good news:
- Very very simple
- Can then simply choose the method with the best test-set score
- Bad news:
- What's the downside?

from Andrew Moore (CMU)

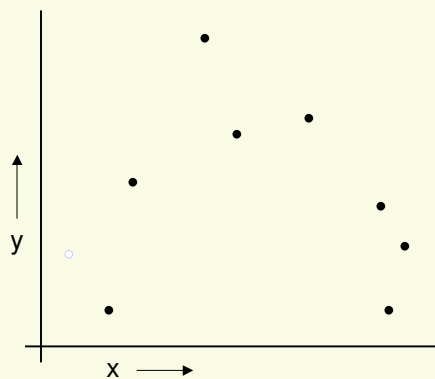
## The test set method

- Good news:
- Very very simple
- Can then simply choose the method with the best test-set score
- Bad news:
- Wastes data: we get an estimate of the best method to apply to 30% less data
  - if we don't have much data, our test-set might just be lucky or unlucky

We say the "test-set estimator of performance has high variance"

from Andrew Moore (CMU)

## LOOCV (Leave-one-out Cross Validation)

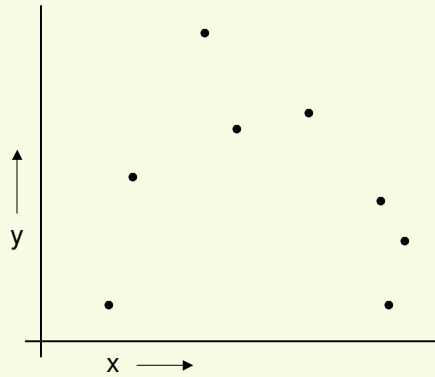


For  $k=1$  to  $R$

1. Let  $(x_k, y_k)$  be the  $k^{\text{th}}$  record

from Andrew Moore (CMU)

## LOOCV (Leave-one-out Cross Validation)

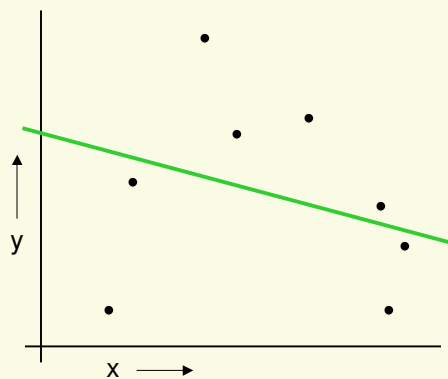


For  $k=1$  to  $R$

1. Let  $(x_k, y_k)$  be the  $k^{\text{th}}$  record
2. Temporarily remove  $(x_k, y_k)$  from the dataset

from Andrew Moore (CMU)

## LOOCV (Leave-one-out Cross Validation)

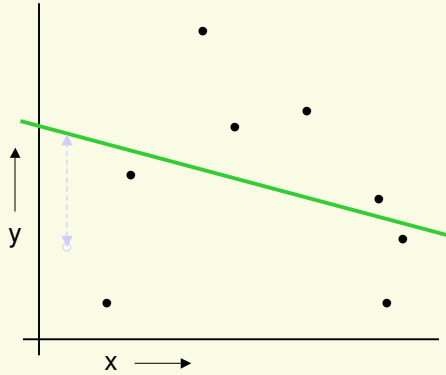


For  $k=1$  to  $R$

1. Let  $(x_k, y_k)$  be the  $k^{\text{th}}$  record
2. Temporarily remove  $(x_k, y_k)$  from the dataset
3. Train on the remaining  $R-1$  datapoints

from Andrew Moore (CMU)

## LOOCV (Leave-one-out Cross Validation)

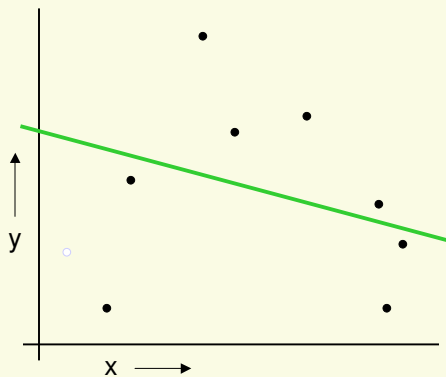


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4. Note your error  $(x_k, y_k)$

from Andrew Moore (CMU)

## LOOCV (Leave-one-out Cross Validation)



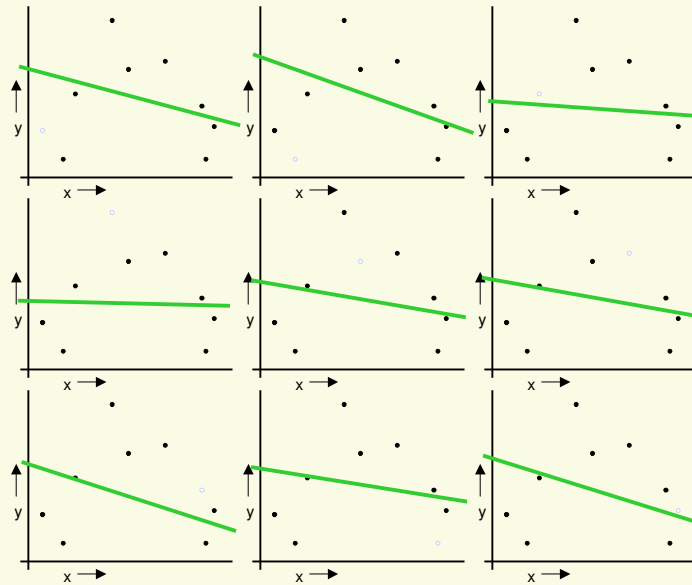
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When you've done all points, report the mean error.

from Andrew Moore (CMU)

## LOOCV (Leave-one-out Cross Validation)



For  $k=1$  to  $R$

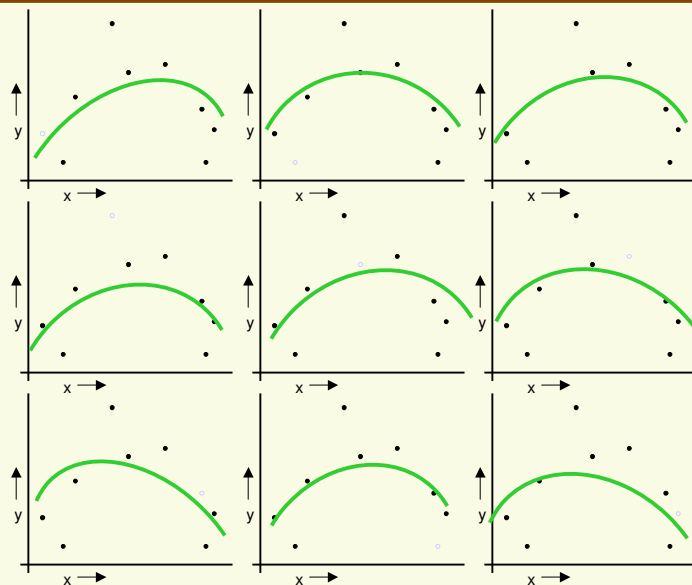
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4. Note your error  $(x_k, y_k)$

When you've done all points, report the mean error.

$$MSE_{LOOCV} = 2.12$$

from Andrew Moore (CMU)

## LOOCV for Quadratic Regression



For  $k=1$  to  $R$

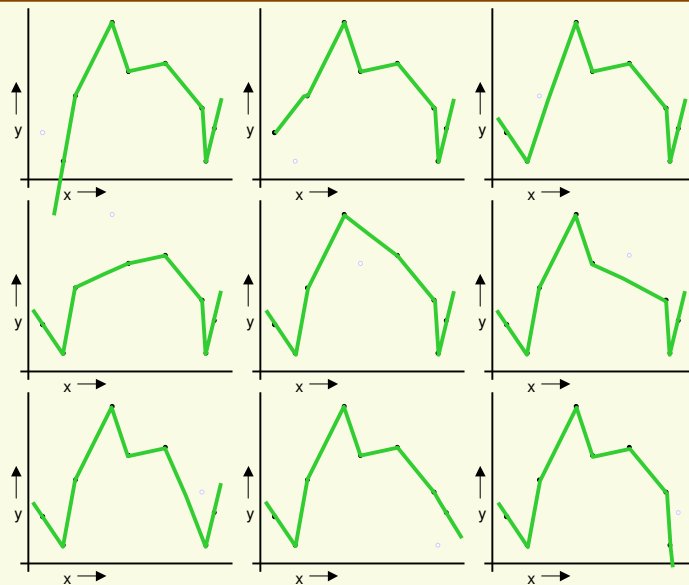
1. Let  $(x_k, y_k)$  be the  $k^{\text{th}}$  record
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3. Train on the remaining  $R-1$  datapoints
4. Note your error  $(x_k, y_k)$

When you've done all points, report the mean error.

$$MSE_{LOOCV} = 0.962$$

from Andrew Moore (CMU)

## LOOCV for Join The Dots



For  $k=1$  to  $R$

1. Let  $(x_k, y_k)$  be the  $k^{\text{th}}$  record
2. Temporarily remove  $(x_k, y_k)$  from the dataset
3. Train on the remaining  $R-1$  datapoints
4. Note your error  $(x_k, y_k)$

When you've done all points, report the mean error.

$$MSE_{LOOCV} = 3.33$$

from Andrew Moore (CMU)

## Which kind of Cross Validation?

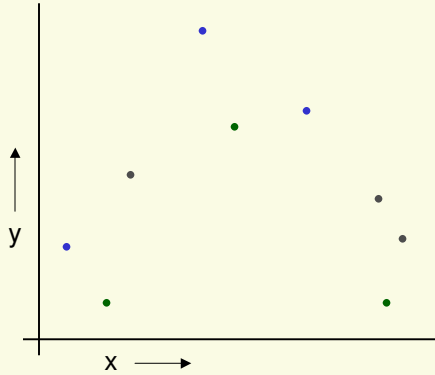
	Downside	Upside
Test-set	Variance: unreliable estimate of future performance	Cheap
Leave-one-out	Expensive	Doesn't waste data

..can we get the best of both worlds?

from Andrew Moore (CMU)

## ***k*-fold Cross Validation**

Randomly break the dataset into  $k$  partitions (in our example we'll have  $k=3$  partitions colored Red Green and Blue)

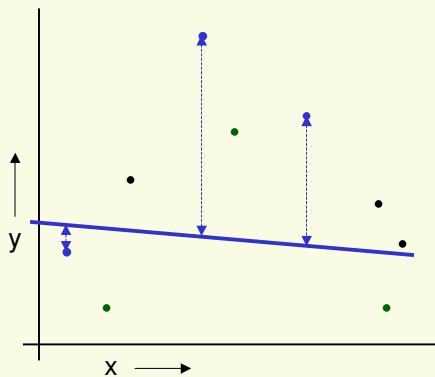


from Andrew Moore (CMU)

## ***k*-fold Cross Validation**

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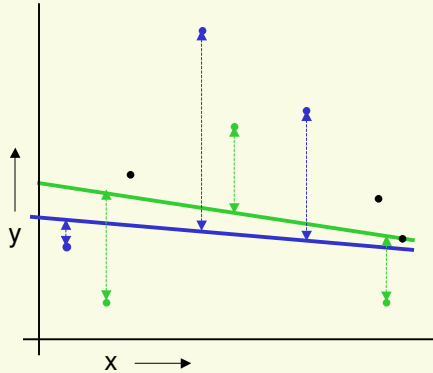
For the blue partition: Train on all the points not in the blue partition. Find the test-set sum of errors on the blue points.



from Andrew Moore (CMU)

## ***k*-fold Cross Validation**

Randomly break the dataset into  $k$  partitions (in our example we'll have  $k=3$  partitions colored Red Green and Blue)



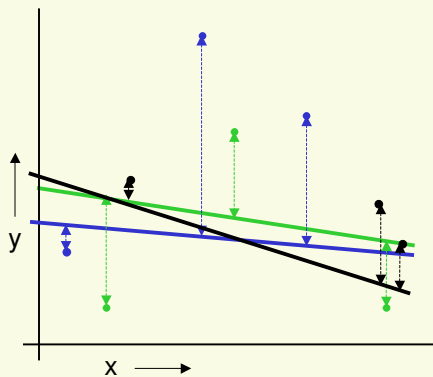
For the blue partition: Train on all the points not in the blue partition. Find the test-set sum of errors on the blue points.

For the green partition: Train on all the points not in the green partition. Find the test-set sum of errors on the green points.

from Andrew Moore (CMU)

## ***k*-fold Cross Validation**

Randomly break the dataset into  $k$  partitions (in our example we'll have  $k=3$  partitions colored Red Green and Blue)



For the blue partition: Train on all the points not in the blue partition. Find the test-set sum of errors on the blue points.

For the green partition: Train on all the points not in the green partition. Find the test-set sum of errors on the green points.

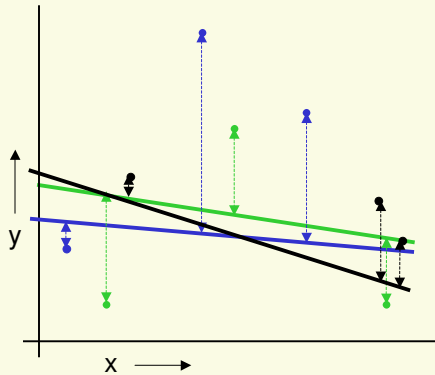
For the gray partition: Train on all the points not in the gray partition. Find the test-set sum of errors on the gray points.

from Andrew Moore (CMU)



## k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Red Green and Blue)



Linear Regression  
 $MSE_{3FOLD}=2.05$

For the blue partition: Train on all the points not in the blue partition. Find the test-set sum of errors on the blue points.

For the green partition: Train on all the points not in the green partition. Find the test-set sum of errors on the green points.

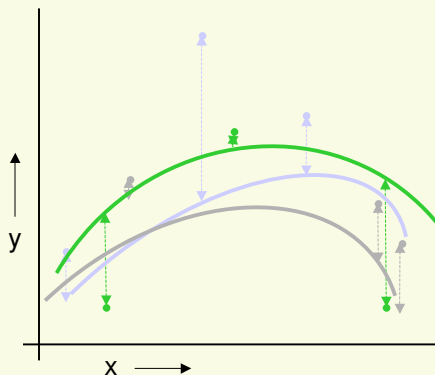
For the gray partition: Train on all the points not in the gray partition. Find the test-set sum of errors on the gray points.

Then report the mean error

from Andrew Moore (CMU)

## k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Red Green and Blue)



Quadratic Regression  
 $MSE_{3FOLD}=1.11$

For the blue partition: Train on all the points not in the blue partition. Find the test-set sum of errors on the blue points.

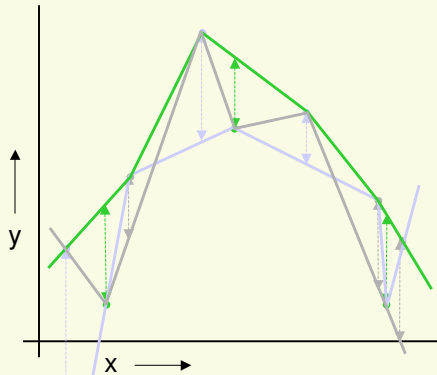
For the green partition: Train on all the points not in the green partition. Find the test-set sum of errors on the green points.

For the gray partition: Train on all the points not in the gray partition. Find the test-set sum of errors on the gray points.

Then report the mean error

from Andrew Moore (CMU)

## k-fold Cross Validation



Joint-the-dots  
 $MSE_{3FOLD}=2.93$

Randomly break the dataset into k partitions (in our example we'll have  $k=3$  partitions colored Red Green and Blue)

For the blue partition: Train on all the points not in the blue partition. Find the test-set sum of errors on the blue points.

For the green partition: Train on all the points not in the green partition. Find the test-set sum of errors on the green points.

For the gray partition: Train on all the points not in the gray partition. Find the test-set sum of errors on the gray points.

Then report the mean error

from Andrew Moore (CMU)












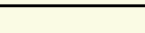
## Which kind of Cross Validation?

	Downside	Upside
<b>Test-set</b>	Variance: unreliable estimate of future performance	Cheap
<b>Leave-one-out</b>	Expensive	Doesn't waste data
<b>10-fold</b>	Wastes 10% of the data. 10 times more expensive than test set	Only wastes 10%. Only 10 times more expensive instead of R times.
<b>3-fold</b>	Wastier than 10-fold. Expensivier than test set	Slightly better than test-set
<b>N-fold</b>	Identical to Leave-one-out	

from Andrew Moore (CMU)

## CV-based Model Selection













- We're trying to decide which algorithm to use.
- We train each machine and make a table...

$i$	$f_i$	TRAINERR	10-FOLD-CV-ERR	Choice
1	$f_1$			
2	$f_2$			
3	$f_3$			⊗
4	$f_4$			
5	$f_5$			
6	$f_6$			

from Andrew Moore (CMU)

## CV-based Model Selection

- Example: Choosing number of hidden units in a one-hidden-layer neural net.
- Step 1: Compute 10-fold CV error for six different model

Algorithm	TRAINERR	10-FOLD-CV-ERR	Choice
0 hidden units			
1 hidden units			
2 hidden units			⊗
3 hidden units			
4 hidden units			
5 hidden units			

- Step 2: Whichever model class gave best CV score: train it with all the data, and that's the predictive model you'll use.

from Andrew Moore (CMU)

## CV-based Model Selection

- Example: Choosing “k” for a k-nearest-neighbor regression.
- Step 1: Compute LOOCV error for six different model classes:

Algorithm	TRAINERR	10-fold-CV-ERR	Choice
K=1			
K=2			
K=3			
K=4			☒
K=5			
K=6			

- Step 2: Whichever model class gave best CV score: train it with all the data, and that’s the predictive model you’ll use.

from Andrew Moore (CMU)

## CV-based Model Selection

- Example: Choosing “k” for a k-nearest-neighbor regression.
- Step 1: Compute LOOCV error for six different model classes:

Algorithm	TRAINERR	10-fold-CV-ERR	Choice
K=1			
K=2			
K=3			
K=4			☒
K=5			
K=6			

Why did we use 10-fold-CV for neural nets and LOOCV for k-nearest neighbor?

And why stop at K=6

Are we guaranteed that a local optimum of K vs LOOCV will be the global optimum?

What should we do if we are depressed at the expense of doing LOOCV for K= 1 through 1000?

The reason is Computational. For k-NN (and all other nonparametric methods) LOOCV happens to be as cheap as regular predictions.

No good reason, except it looked like things were getting worse as K was increasing

Sadly, no. And in fact, the relationship can be very bumpy.

Idea One: K=1, K=2, K=4, K=8, K=16, K=32, K=64 ... K=1024

Idea Two: Hillclimbing from an initial guess at K

- Step 2: Whichever model class gave best CV score: train it with all the data, and that’s the predictive model you’ll use.

from Andrew Moore (CMU)

## ***CV-based Model Selection***

---

- Can you think of other decisions we can ask Cross Validation to make for us, based on other machine learning algorithms in the class so far?

from Andrew Moore (CMU)

## ***CV-based Model Selection***

---

- Can you think of other decisions we can ask Cross Validation to make for us, based on other machine learning algorithms in the class so far?
  - Degree of polynomial in polynomial regression
  - Whether to use full, diagonal or spherical Gaussians in a Gaussian Bayes Classifier.
  - The Kernel Width in Kernel Regression
  - The Kernel Width in Locally Weighted Regression
  - The Bayesian Prior in Bayesian Regression

These involve  
choosing the value of a  
real-valued parameter.  
What should we do?

from Andrew Moore (CMU)

## CV-based Model Selection

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These involve choosing the value of a real-valued parameter. What should we do?

Idea One: Consider a discrete set of values (often best to consider a set of values with exponentially increasing gaps, as in the K-NN example).

Idea Two: Compute  $\frac{\partial \text{LOOCV}}{\partial \text{Parameter}}$  and then do gradient descent.

from Andrew Moore (CMU)

## CV-based Model Selection

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Idea Two: Compute  $\frac{\partial \text{LOOCV}}{\partial \text{Parameter}}$  and then do gradient descent.

from Andrew Moore (CMU)

## CV-based Algorithm Choice

- Example: Choosing which regression algorithm to use
- Step 1: Compute 10-fold-CV error for six different model classes:

Algorithm	TRAINERR	10-fold-CV-ERR	Choice
1-NN			
10-NN			
Linear Reg'n			
Quad reg'n			<input checked="" type="checkbox"/>
LWR, KW=0.1			
LWR, KW=0.5			

- Step 2: Whichever algorithm gave best CV score: train it with all the data, and that's the predictive model you'll use.

from Andrew Moore (CMU)

## Cross-validation for classification

- Instead of computing the sum squared errors on a test set, you should compute...

from Andrew Moore (CMU)

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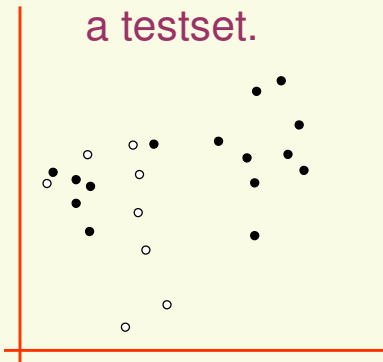
The total number of misclassifications on a testset.

from Andrew Moore (CMU)

## Cross-validation for classification

- Instead of computing the sum squared errors on a test set, you should compute...

The total number of misclassifications on a testset.



- What's LOOCV of 1-NN?
- What's LOOCV of 3-NN?
- What's LOOCV of 22-NN?

from Andrew Moore (CMU)



## ***Cross-Validation for classification***

---

- Choosing  $k$  for  $k$ -nearest neighbors
- Choosing  $h$  for the Parzen windows
- Any other “free” parameter of a classifier
- Choosing which classifier to use
- Choosing Features to use

from Andrew Moore (CMU)

## ***Feature Selection***

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- Suppose you have a learning algorithm LA and a set of input attributes  $\{X_1, X_2 \dots X_m\}$
- You expect that LA will only find some subset of the attributes useful.
- Question: How can we use cross-validation to find a useful subset?
- Four ideas:
  - Forward selection
  - Backward elimination
  - Hill Climbing
  - Stochastic search (Simulated Annealing or GAs)

Another fun area in which Andrew has spent a lot of his wild youth

from Andrew Moore (CMU)

## ***Ensemble Learning: Bagging and Boosting***

- So far we have talked about design of a single classifier that generalizes well (want to “learn”  $f(x)$  )
- From statistics, we know that it is good to average your predictions (reduces variance)
- Bagging
  - reshuffle your training data to create  $k$  different training sets and learn  $f_1(x), f_2(x), \dots, f_k(x)$
  - Combine the  $k$  different classifiers by majority voting
$$f_{\text{FINAL}}(x) = \text{sign}[\sum 1/k f_i(x) ]$$
- Boosting
  - Assign different weights to training samples in a “smart” way so that different classifiers pay more attention to different samples
  - Weighted majority voting, the weight of individual classifier is proportional to its accuracy
  - Ada-boost (1996) was influenced by bagging, and it is superior to bagging

## ***Bagging***

- Generate a random sample from training set by selecting  $l$  elements (out of  $n$  elements available) with replacement
- each classifier is trained on the average of 63.2% of the training examples
  - For a dataset with  $N$  examples, each example has a probability of  $1-(1-1/N)^N$  of being selected at least once in the  $N$  samples. For  $N \rightarrow \infty$ , this number converges to  $(1-1/e)$  or 0.632 [Bauer and Kohavi, 1999]
- Repeat the sampling procedure, getting a sequence of  $k$  independent training sets
- A corresponding sequence of classifiers  $f_1(x), f_2(x), \dots, f_k(x)$  is constructed for each of these training sets, using the same classification algorithm
- To classify an unknown sample  $x$ , let each classifier predict.
- The *bagged classifier*  $f_{\text{FINAL}}(x)$  then combines the predictions of the individual classifiers to generate the final outcome, frequently this combination is simple voting

## ***Boosting: motivation***

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- It is usually hard to design an accurate classifier which generalizes well
- However it is usually easy to find many “rule of thumb” *weak* classifiers
  - A classifier is weak if it is only slightly better than random guessing
- Can we combine several weak classifiers to produce an accurate classifier?
  - Question people have been working on since 1980's

## ***Ada Boost***

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- Let's assume we have 2-class classification problem, with  $y_i \in \{-1, 1\}$
- Ada boost will produce a discriminant function:

$$g(x) = \sum_{t=1}^T \alpha_t f_t(x)$$

- where  $f_t(x)$  is the “weak” classifier
- As usual, the final classifier is the sign of the discriminant function, that is  $f_{\text{final}}(x) = \text{sign}[g(x)]$

## ***Idea Behind Ada Boost***

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- Algorithm is iterative
- Maintains distribution of weights over the training examples
- Initially distribution of weights is uniform
- At successive iterations, the weight of misclassified examples is increased, forcing the weak learner to focus on the hard examples in the training set

## ***More Comments on Ada Boost***

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- Ada boost is very simple to implement, provided you have an implementation of a “weak learner”
- Will work as long as the “basic” classifier  $f_t(x)$  is at least slightly better than random
  - will work if the error rate of  $f_t(x)$  is less than 0.5 (0.5 is the error rate of a random guessing classifier for a 2-class problem)
- Can be applied to boost any classifier, not necessarily weak

## Ada Boost (slightly modified from the original version)

- $d(x)$  is the distribution of weights over the  $N$  training points  $\sum d(x_i)=1$
- Initially assign uniform weights  $d_0(x_i) = 1/N$  for all  $x_i$
- At each iteration  $t$  :
  - Find best weak classifier  $f_t(x)$  using weights  $d_t(x)$
  - Compute the error rate  $\epsilon_t$  as
$$\epsilon_t = \sum_{i=1 \dots N} d_t(x_i) \cdot \mathbb{I}[y_i \neq f_t(x_i)]$$
  - assign weight  $\alpha_t$  the classifier  $f_t$ 's in the final hypothesis
$$\alpha_t = \log((1 - \epsilon_t)/\epsilon_t)$$
  - For each  $x_i$ ,  $d_{t+1}(x_i) = d_t(x_i) \cdot \exp[\alpha_t \cdot \mathbb{I}(y_i \neq f_t(x_i))]$
  - Normalize  $d_{t+1}(x_i)$  so that  $\sum_{i=1} d_{t+1}(x_i) = 1$
- $f_{FINAL}(x) = \text{sign} [ \sum \alpha_t f_t(x) ]$

## Ada Boost

- At each iteration  $t$  :
  - Find best weak classifier  $f_t(x)$  using weights  $d_t(x)$
  - Compute  $\epsilon_t$  the error rate as
$$\epsilon_t = \sum d_t(x_i) \cdot \mathbb{I}[y_i \neq f_t(x_i)]$$
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  - Normalize  $d_{t+1}(x_i)$  so that  $\sum_{t+1} d(x_i) = 1$
- $f_{FINAL}(x) = \text{sign} [ \sum \alpha_t f_t(x) ]$
- If the classifier does not take weighted samples, this step can be achieved by sampling from the training samples according to the distribution  $d_t(x)$

## Ada Boost

- At each iteration  $t$  :
  - Find best weak classifier  $f_t(x)$  using weights  $d_t(x)$
  - Compute  $\epsilon_t$  the error rate as
$$\epsilon_t = \sum d_t(x_i) \cdot \mathbb{1}[y_i \neq f_t(x_i)]$$
  - assign weight  $\alpha_t$  the classifier  $f_t$ 's in the final hypothesis
$$\alpha_t = \log((1 - \epsilon_t)/\epsilon_t)$$
  - For each  $x_i$ ,  $d_{t+1}(x_i) = d_t(x_i) \cdot \exp[\alpha_t \cdot \mathbb{1}(y_i \neq f_t(x_i))]$
  - Normalize  $d_{t+1}(x_i)$  so that  $\sum d_{t+1}(x_i) = 1$
  - $f_{FINAL}(x) = \text{sign} [ \sum \alpha_t f_t(x) ]$
- Since the weak classifier is better than random, we expect  $\epsilon_t < 1/2$

## Ada Boost

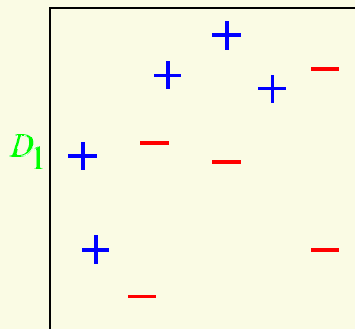
- At each iteration  $t$  :
  - Find best weak classifier  $f_t(x)$  using weights  $d_t(x)$
  - Compute  $\epsilon_t$  the error rate as
$$\epsilon_t = \sum d_t(x_i) \cdot \mathbb{1}(y_i \neq f_t(x_i))$$
  - assign weight  $\alpha_t$  the classifier  $f_t$ 's in the final hypothesis
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  - For each  $x_i$ ,  $d_{t+1}(x_i) = d_t(x_i) \cdot \exp[\alpha_t \cdot \mathbb{1}(y_i \neq f_t(x_i))]$
  - Normalize  $d_{t+1}(x_i)$  so that  $\sum d_{t+1}(x_i) = 1$
  - $f_{FINAL}(x) = \text{sign} [ \sum \alpha_t f_t(x) ]$
- Recall that  $\epsilon_t < 1/2$
- Thus  $(1 - \epsilon_t)/\epsilon_t > 1 \Rightarrow \alpha_t > 0$
- The smaller is  $\epsilon_t$ , the larger is  $\alpha_t$ , and thus the more importance (weight) classifier  $f_t(x)$  gets in the final classifier
$$f_{FINAL}(x) = \text{sign} [ \sum \alpha_t f_t(x) ]$$

## Ada Boost

- At each iteration  $t$  :
  - Find best weak classifier  $f_t(x)$  using weights  $d_t(x)$
  - Compute  $\epsilon_t$  the error rate as
$$\epsilon_t = \sum d_t(x_i) \cdot I(y_i \neq f_t(x_i))$$
  - assign weight  $\alpha_t$  the classifier  $f_t$ 's in the final hypothesis
$$\alpha_t = \log((1 - \epsilon_t)/\epsilon_t)$$
  - For each  $x_i$ ,  $d_{t+1}(x_i) = d_t(x_i) \cdot \exp[\alpha_t \cdot I(y_i \neq f_t(x_i))]$
  - Normalize  $d_{t+1}(x_i)$  so that  $\sum d_{t+1}(x_i) = 1$
- $f_{FINAL}(x) = \text{sign}[\sum \alpha_t f_t(x)]$
- Weight of misclassified examples is increased and the new  $d_{t+1}(x_i)$ 's are normalized to be a distribution again

## AdaBoost Example

from "A Tutorial on Boosting" by Yoav Freund and Rob Schapire

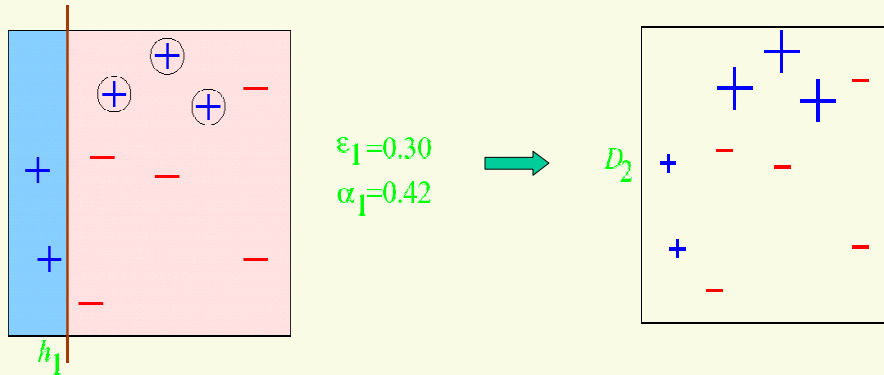


Original Training set : equal weights to all training samples

Note: in the following slides,  $h_t(x)$  is used instead of  $f_t(x)$ , and  $D$  instead of  $d$

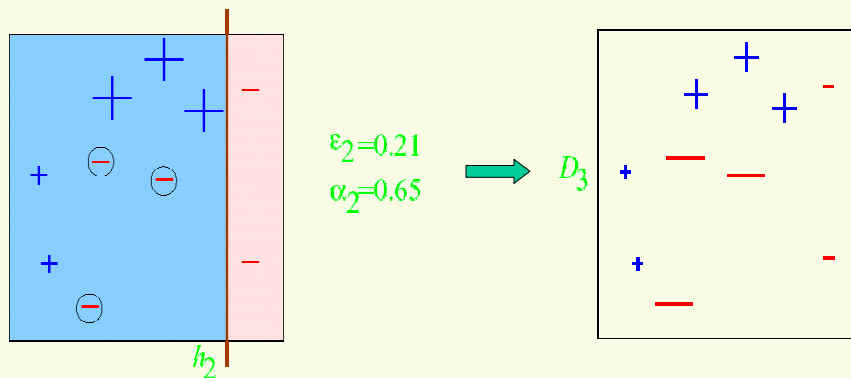
## AdaBoost Example

ROUND 1



## AdaBoost Example

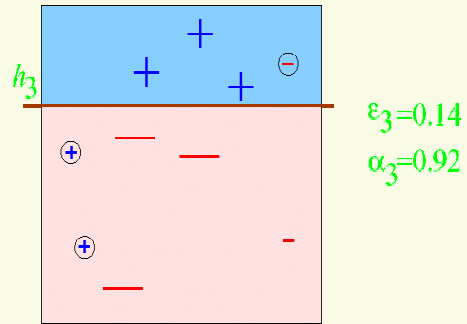
ROUND 2





## AdaBoost Example

ROUND 3



## AdaBoost Example

$$f_{\text{FINAL}}(x) = \text{sign} \left( 0.42 \left( \begin{array}{|c|} \hline \text{blue} \\ \hline \text{pink} \end{array} \right) + 0.65 \left( \begin{array}{|c|} \hline \text{blue} \\ \hline \text{pink} \end{array} \right) + 0.92 \left( \begin{array}{|c|} \hline \text{blue} \\ \hline \text{pink} \end{array} \right) \right)$$

$$= \begin{array}{|c|} \hline \text{blue} \\ \hline \text{pink} \end{array}$$

## AdaBoost Comments

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- It can be shown that the training error drops exponentially fast, if each weak classifier is slightly better than random

$$Err_{train} \leq \exp\left(-2\sum_t \gamma_t^2\right)$$

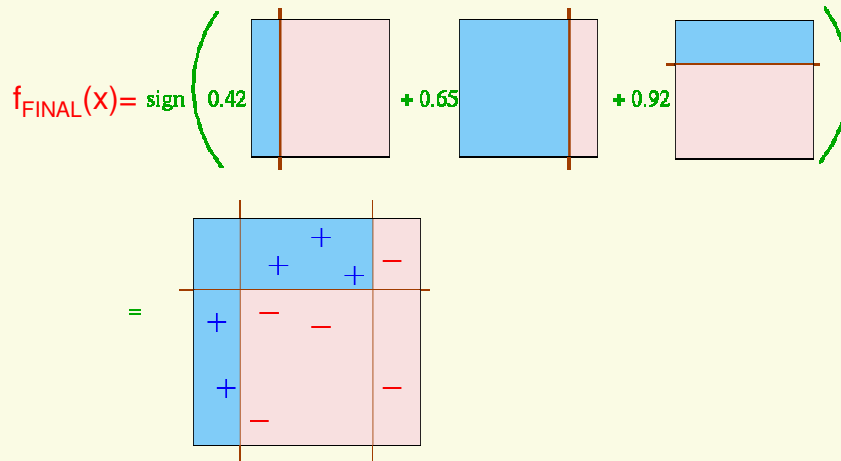
- Here  $\gamma_t = \epsilon_t - 1/2$ , where  $\epsilon_t$  is classification error at round  $t$  (weak classifier  $f_t$ )

## AdaBoost Comments

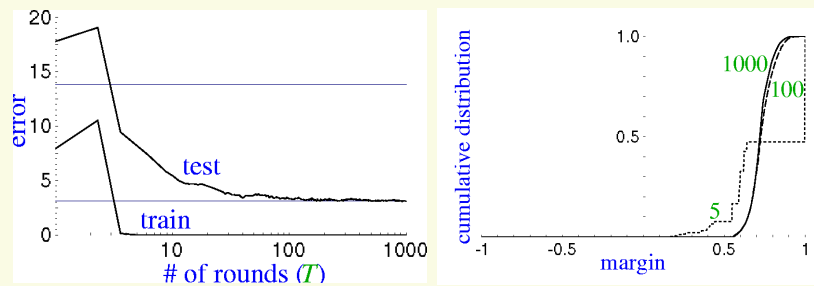
---

- But we are really interested in the generalization properties of  $f_{FINAL}(x)$ , not the training error
- AdaBoost was shown to have excellent generalization properties in practice
  - the more rounds, the more complex is the final classifier, so overfitting is expected as the training proceeds
  - but in the beginning researchers observed no overfitting of the data
  - It turns out it does overfit data eventually, if you run it really long
- It can be shown that boosting “aggressively” increases the margins of training examples, as iterations proceed
  - margins continue to increase even when training error reaches zero
  - Helps to explain empirically observed phenomena: test error continues to drop even after training error reaches zero

## AdaBoost Example



## The Margin Distribution



epoch	5	100	1000
training error	0.0	0.0	0.0
test error	8.4	3.3	3.1
%margins $\leq 0.5$	7.7	0.0	0.0
Minimum margin	0.14	0.52	0.55

## Boosting As Additive Model

- The final prediction in boosting  $g(x)$  can be expressed as an **additive expansion** of individual classifiers

$$g(x) = \sum_{k=1}^M \alpha_k f_k(x; \gamma_k)$$

- Typically we would try to **minimize a loss function** on the  $N$  training examples

$$\min_{\alpha_1, \gamma_1, \dots, \gamma_M, \alpha_M} \sum_{i=1}^N L\left(y_i, \sum_{k=1}^M \alpha_k f_k(x_i; \gamma_k)\right)$$

- For example, under squared-error loss:

$$\min_{\alpha_1, \gamma_1, \dots, \gamma_M, \alpha_M} \sum_{i=1}^N \left(y_i - \sum_{k=1}^M \alpha_k f_k(x_i; \gamma_k)\right)^2$$

## Boosting As Additive Model

- Forward stage-wise modeling is iterative and fits the  $f_k(x, \gamma_k)$  sequentially, fixing the results of previous iterations

$$g_t(x) = \overset{\text{model at iteration } t}{\text{fixed}} g_{t-1}(x) + \overset{\text{fit } \gamma_t, \alpha_t \text{ to produce improved } g_t(x)}{\alpha_t} f_t(x; \gamma_t)$$

- Under the squared difference loss function:

$$\begin{aligned} L(y_i, g_{t-1}(x_i) + \alpha_t f_t(x_i; \gamma_t)) &= \\ &= (y_i - \underset{\text{fixed}}{g_{t-1}(x_i)} - \alpha_t f_t(x_i; \gamma_t))^2 \end{aligned}$$

- Forward stage-wise optimization seems to produce classifier with better generalization, doing the process stagewise seems to overfit less quickly

## Boosting As Additive Model

$$g(\mathbf{x}) = \sum_{k=1}^M \alpha_k f_k(\mathbf{x}; \gamma_k)$$

- It can be shown that AdaBoost uses forward stage-wise modeling under the following loss function:
  - $L(y, g(x)) = \exp(-y \cdot g(x))$  -- the exponential loss function
  - At stage (or iteration)  $m$ , we fit:

$$\begin{aligned} \arg \min_{\alpha_m, f_m} \sum_{i=1}^N L(y_i, g(x_i)) &= \\ &= \arg \min_{\alpha_m, f_m} \sum_{i=1}^N \exp(-y_i \cdot [g_{m-1}(x_i) + \alpha_m \cdot f_m(x_i)]) \\ &= \arg \min_{\alpha_m, f_m} \sum_{i=1}^N \exp(-y_i \cdot g_{m-1}(x_i)) \cdot \exp(-y_i \cdot \alpha_m \cdot f_m(x_i)) \end{aligned}$$

## Exponential Loss vs. Squared Error Loss

- $L(y, g(x)) = \exp(-y \cdot g(x))$
- $L(y, g(x)) = (y - g(x))^2$



- Squared Error Loss penalizes classifications that are “too correct”, with  $y \cdot g(x) > 1$ , and thus it is inappropriate for classification
- Exponential loss encourages large margins, want  $y \cdot g(x)$  large

## ***Logistic Regression Model***

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- It can be shown that Adaboost builds a logistic regression model:

$$g(x) = \log \frac{\Pr(Y = 1 | x)}{\Pr(Y = -1 | x)} = \sum_{k=1}^M \alpha_k f_k(x)$$

- It can also be shown that the the training error on the samples is at most:

$$\sum_{i=1}^N \exp(-y_i \cdot g(x_i)) = \sum_{i=1}^N \exp\left(-y_i \cdot \sum_{k=1}^M \alpha_k f_k(x_i)\right)$$

## ***Practical Advantages of AdaBoost***

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- fast
- simple
- Has only one parameter to tune ( $T$ )
- flexible: can be combined with any classifier
- provably effective (assuming weak learner)
  - shift in mind set: goal now is merely to find hypotheses that are better than random guessing
- finds outliers
  - The hardest examples are frequently the “outliers”

## ***Caveats***

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- performance depends on data & weak learner
- AdaBoost can fail if
  - weak hypothesis too complex (overfitting)
  - weak hypothesis too weak ( $\gamma_t \rightarrow 0$  too quickly),
    - underfitting
    - Low margins  $\rightarrow$  overfitting
- empirically, AdaBoost seems especially susceptible to noise