CMSC 726
Lecture 13:Evaluation

Lise Getoor

October 14, 2010

ACKNOWLEDGEMENTS: The material in this course is a [illegible] materials from many sources, including: Hal Daume III, Tom Dietterich, Mark Drezde, Carlos Guestrin, **Andrew Moore**, Andrew Ng, Ben Taskar, Eric Xing, and others. I am very grateful for their generous sharing of insights and materials.

Outline

- Evaluating Hypotheses & Learning Algorithms
  - Performance Criteria
  - Motivation
  - Cross Validation
  - Confidence Intervals
- Bias-Variance Decomposition for Regression
- Summary and Conclusion

Evaluating Models

- Need a measure of value – the cost (loss, utility) of a model
- Often use accuracy (or error)
  - Accuracy – how many examples we get “right”
  - Error – how many examples we get wrong
- Can be weighted
  - If examples are not equal, could count the cost (or utility) of mispredicted (correct) examples

Supervised Learning Performance Criteria

- Accuracy/Squared Error/Probability Calibration
- Others:
  - Area under the ROC Curve
  - Lift
  - F-Score
  - Average Precision
  - Precision/Recall Break-Even Point
  - Confusion Matrixes

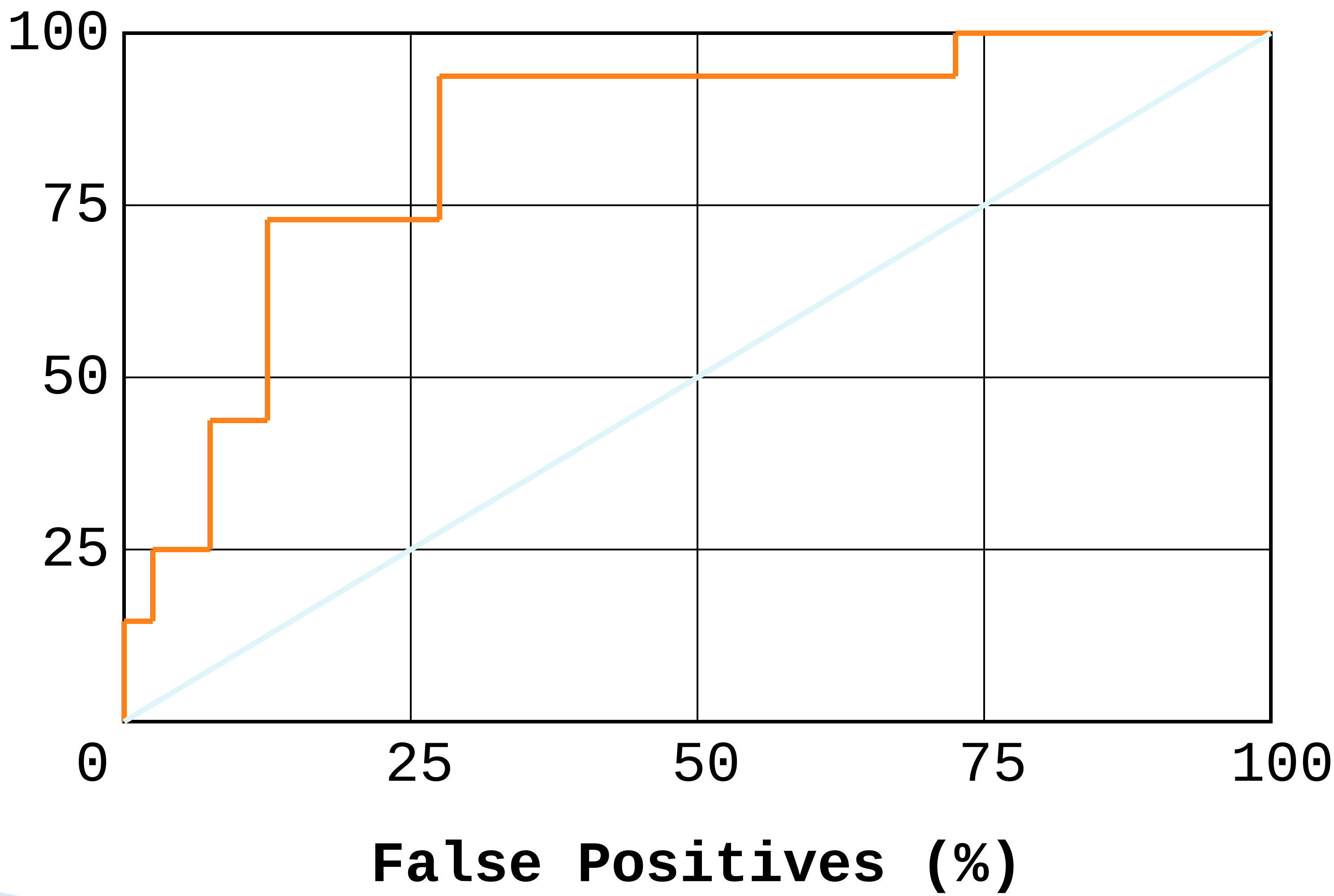
Types of Performance Criteria for Supervised Learning

- Interpret as threshold
  - classification accuracy
- Interpret as probabilities
  - (conditional) likelihood, squared error
- Interpret as ranking
  - ROC curves

Receiver Operator Characteristic (ROC) Curves

- Originally from signal detection
- Becoming very popular for ML
- Used in:
  - Two class problems
  - Where predictions are ordered in some way (e.g., neural network activation is often taken as an indication of how strong or weak a prediction is)
- Plotting an ROC curve:
  - Sort predictions by their predicted strength
  - Start at the bottom left
  - For each positive example, go up 1/P units where P is the number of positive examples
  - For each negative example, go right 1/N units where N is the number of negative examples

ROC Curve



ROC Properties

- Can visualize the tradeoff between coverage and accuracy (as we lower the threshold for prediction how many more true positives will we get in exchange for more false positives)
- Gives a better feel when comparing algorithms
  - Algorithms may do well in different portions of the curve
- A perfect curve would start in the bottom left, go to the top left, then over to the top right
  - A random prediction curve would be a line from the bottom left to the top right
- When comparing curves:
  - Can look to see if one curve dominates the other (is always better)
  - Can compare the area under the curve (very popular – some people even do t-tests on these numbers)

Lift

- Lift measures how much better a classifier is at predicting positives than a baseline classifier that randomly predicts positives (at the rate observed for positives in the data)

$$\text{LIFT} = \frac{\%\ \text{of true positives about the threshold}}{\%\ \text{of dataset about the threshold}}$$

Precision/Recall

- Precision: fraction of examples predicted as positive that are actually positive
- Recall: fraction of true positives that are predicted as positives
- Combining measures:
  - precision-recall F score: harmonic mean of the precision and recall at a given threshold
  - precision at recall level: set recall, measure precision
  - break even point: the precision at which the precision equals recall
  - average precision: average of the precisions at eleven evenly spaced recall levels.

Confusion Matrix

		Predicted		
		Positive	Negative	Total
Actual	Positive	True Positive (TP)	False Negative (FN)	#Positives
	Negative	False Positive (FP)	True Negative (TN)	#Negatives
	Total	TP+FP	FN+TN	#Examples

- Accuracy = (TP+TN) / #Examples
- Error = (FP+FN) / #Examples
- Recall (sensitivity, true positive rate) = TP / #Positives
- Precision = TP / (FP+TP)
- True Negative Rate (specificity) = TN / #Negatives
- False Positive Rate = FP / (FP+TP)
- False Negative Rate = FN / #Negatives

Confusion Matrix – Multi Class

- For many problems (especially multiclass problems), often useful to examine the sources of error
- Confusion matrix:

		Predicted			
		ClassA	ClassB	ClassC	Total
Expected	ClassA	25	5	20	50
	ClassB	0	45	5	50
	ClassC	25	0	25	50
	Total	50	50	50	150

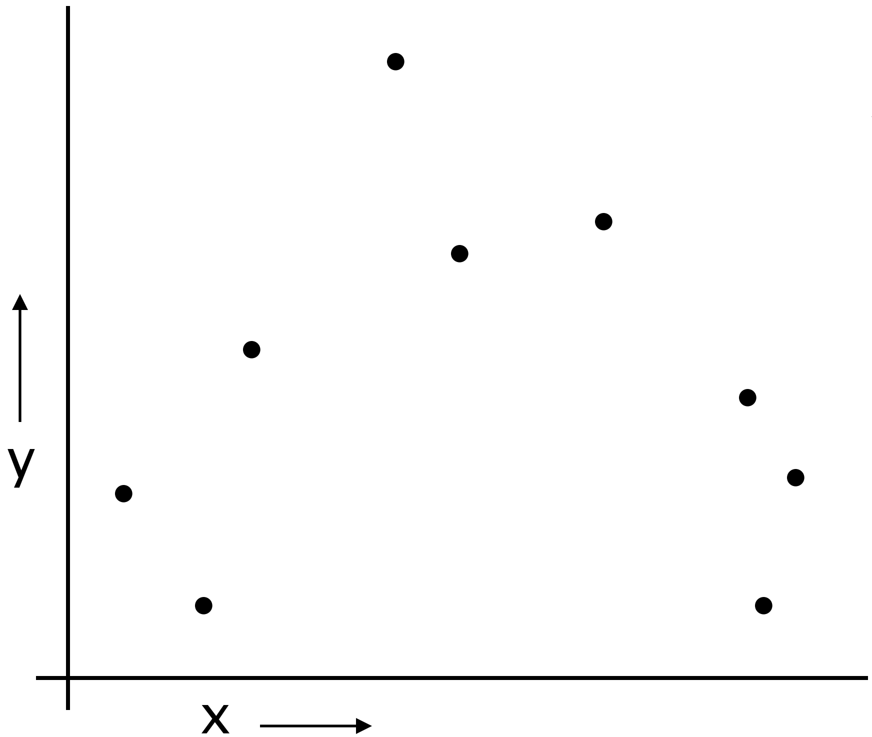
Results Analysis: Confusion Matrix

- Building a confusion matrix
  - Zero all entries
  - For each data point add one in row corresponding to actual class of problem under column corresponding to predicted class
- Perfect prediction has all non-zeros values down the diagonal
- Off diagonal entries can often tell us about what is being mispredicted

Outline

- Evaluating Hypotheses & Learning Algorithms
  - Performance Criteria
  - **Motivation**
  - Cross Validation
  - Confidence Intervals
- Bias-Variance Decomposition for Regression
- Summary and Conclusion

Motivation: A Regression Problem

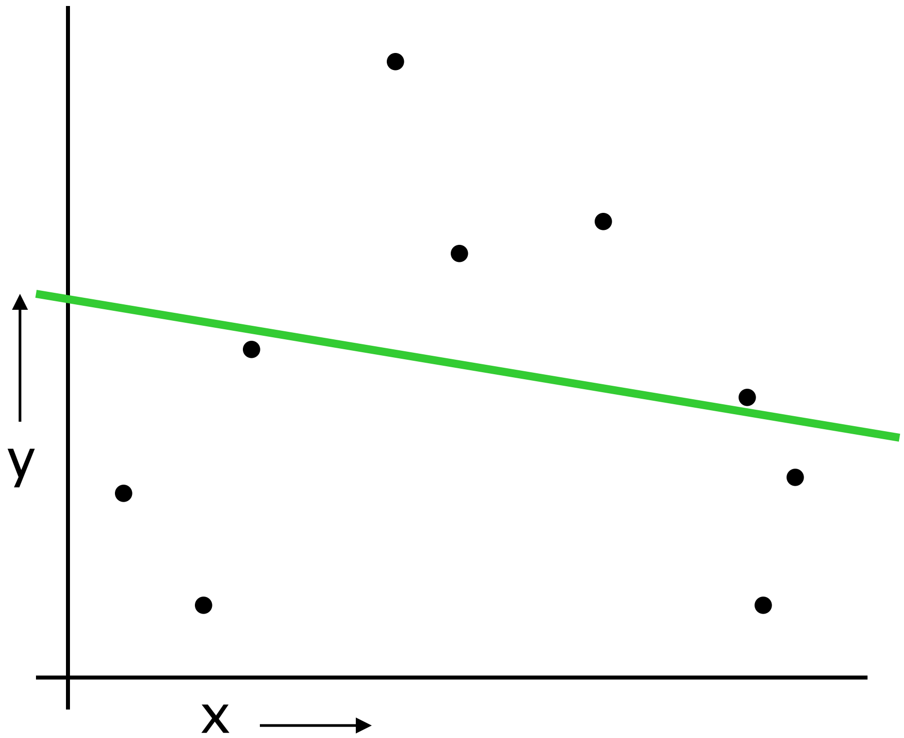


$y = f(x) + \text{noise}$

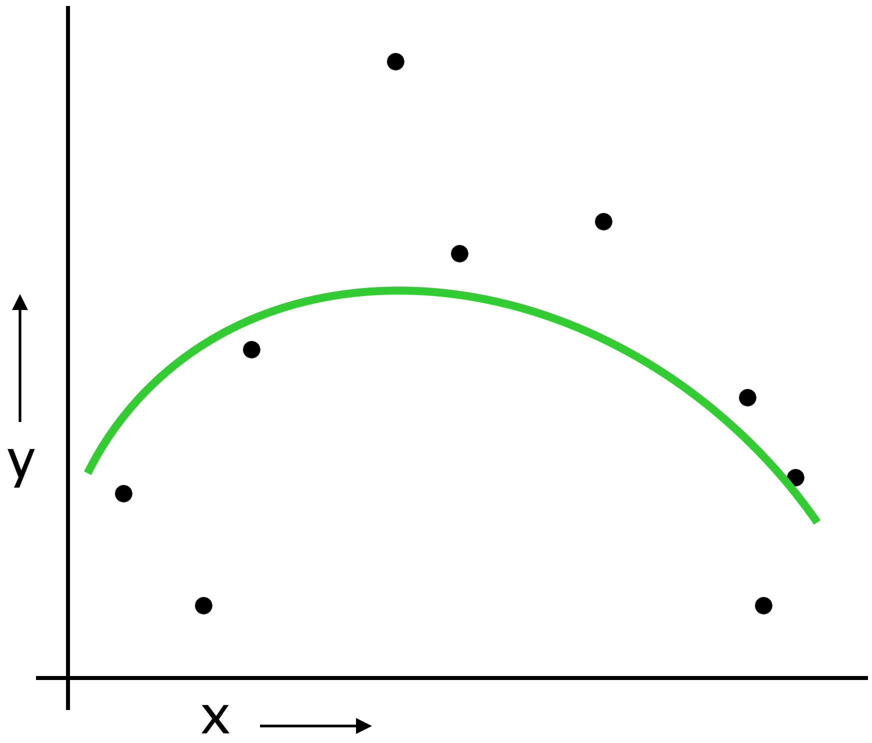
Can we learn f from this data?

Let's consider three methods…

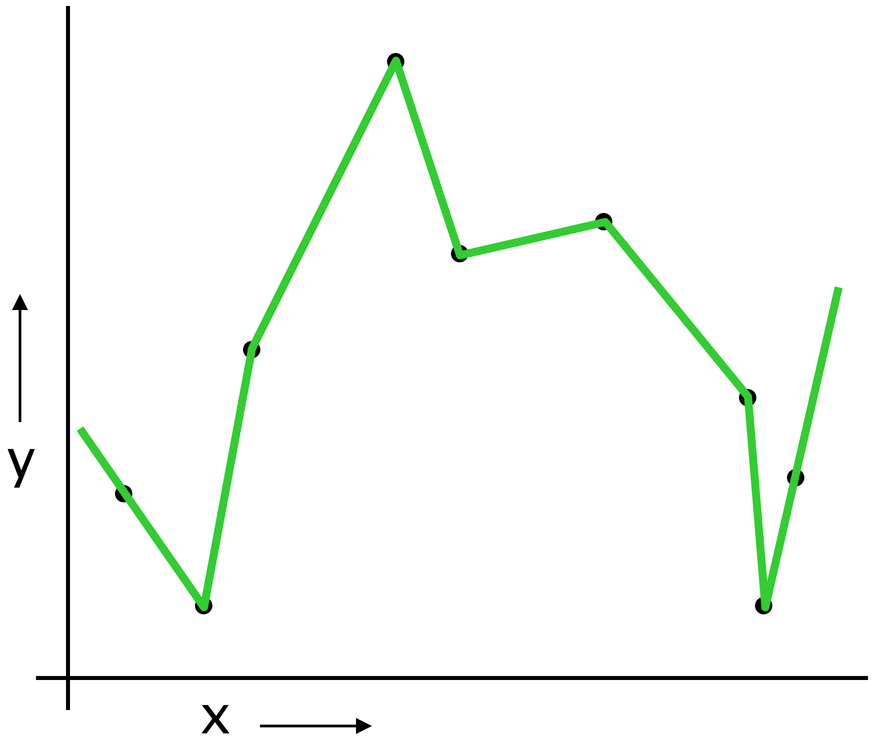
Linear Regression



Quadratic Regression

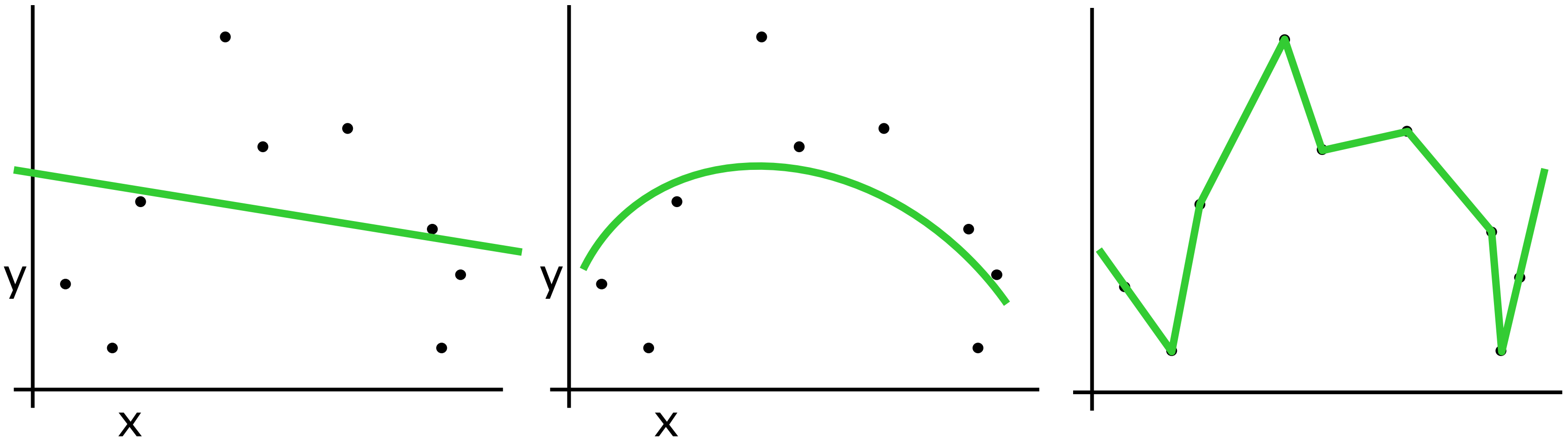


Join-the-dots



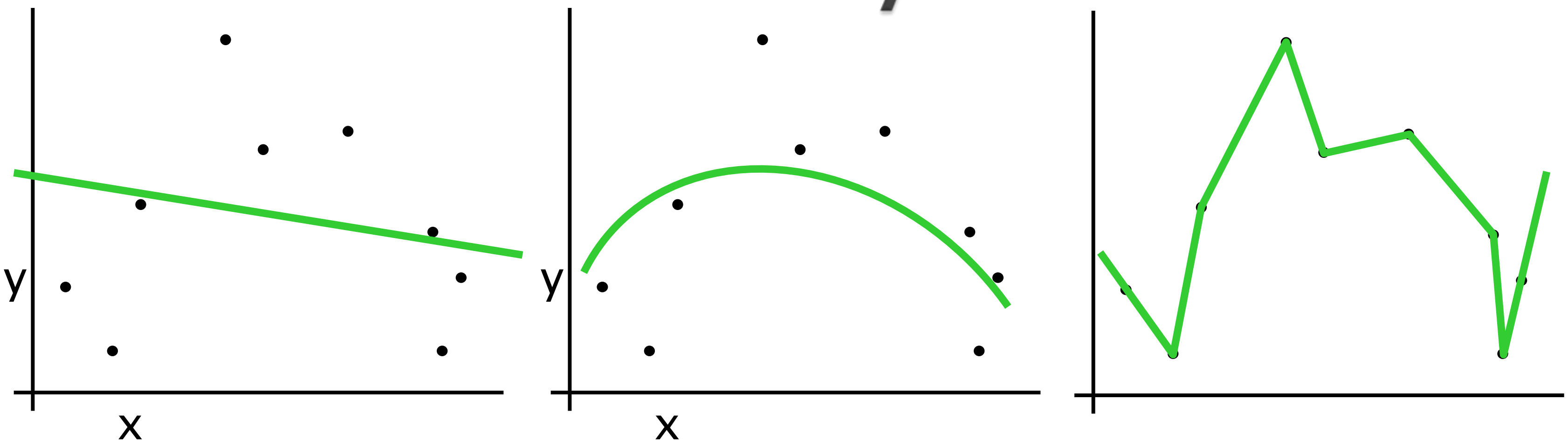
Also known as **piecewise linear nonparametric regression** if you think that sounds better

Which is best?



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

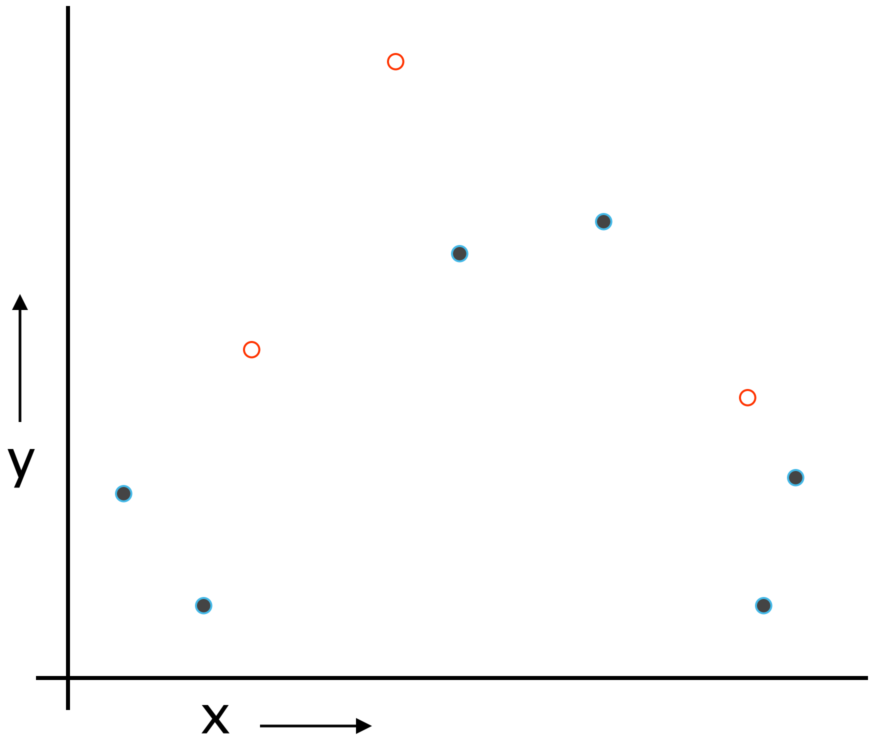
What do we really want?



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?"

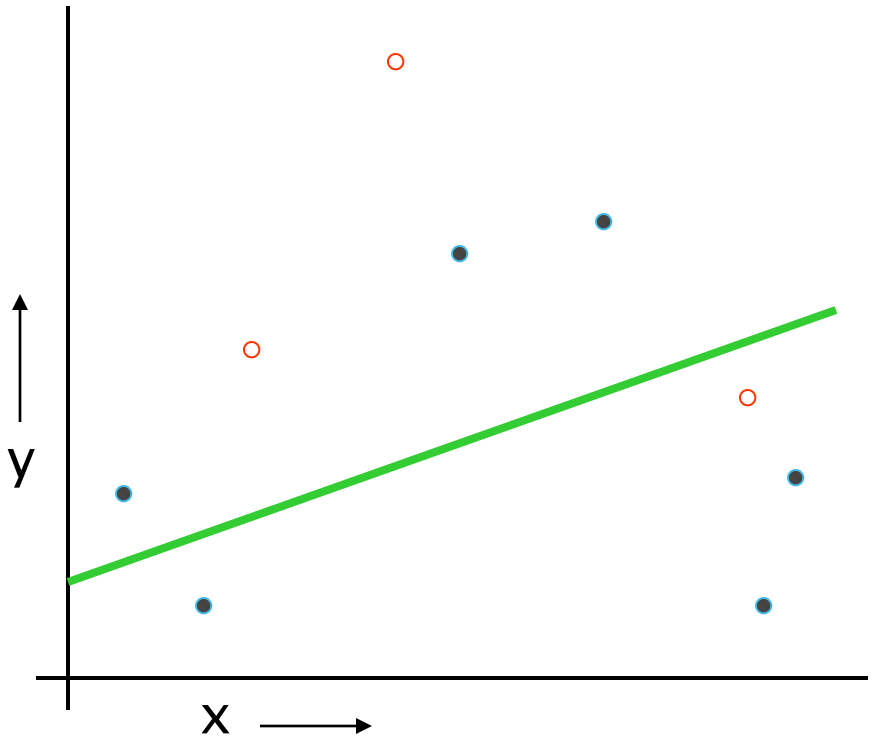
The test set method



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

2. The remainder is a training set

The test set method



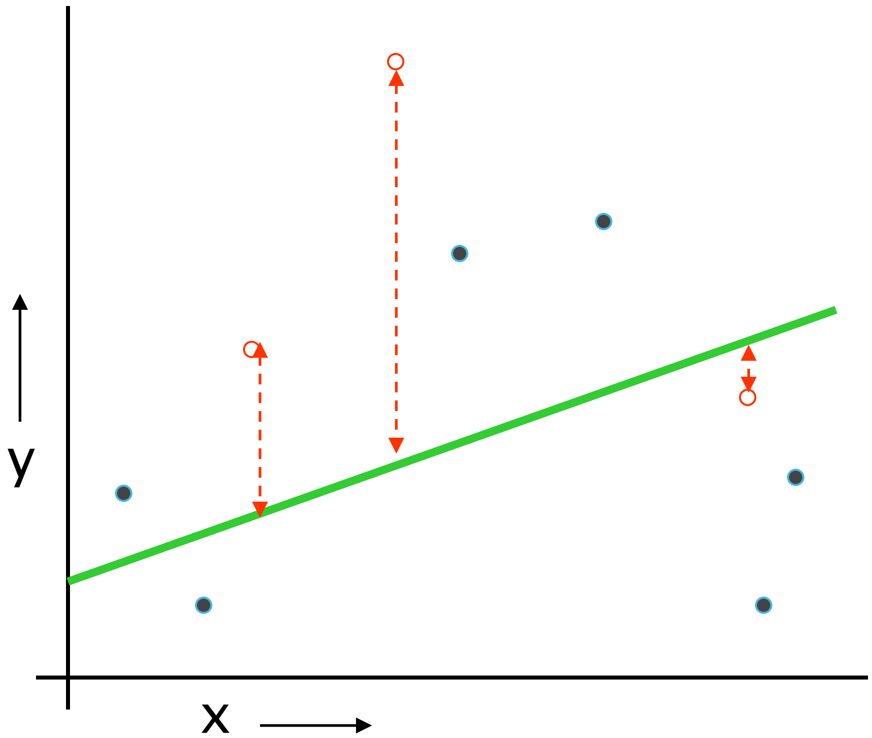
1. Randomly choose 30% of the data to be in a test set

2. The remainder is a training set

3. Perform your regression on the training set

(Linear regression example)

The test set method



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

2. The remainder is a training set

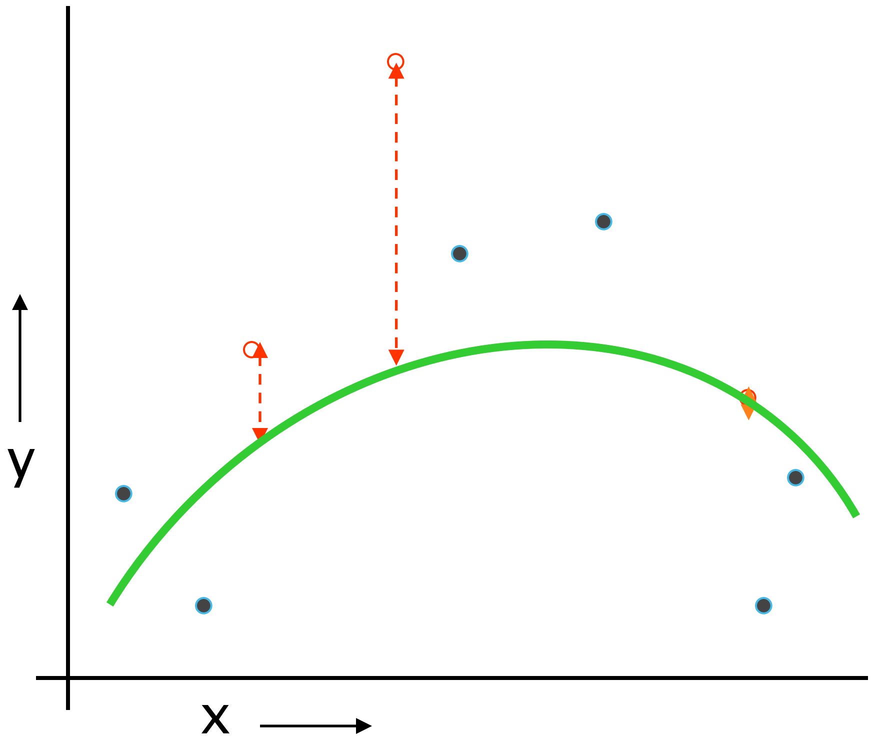
3. Perform your regression on the training set

4. Estimate your future performance with the test set

(Linear regression example)

Mean Squared Error = 2.4

The test set method



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

2. The remainder is a training set

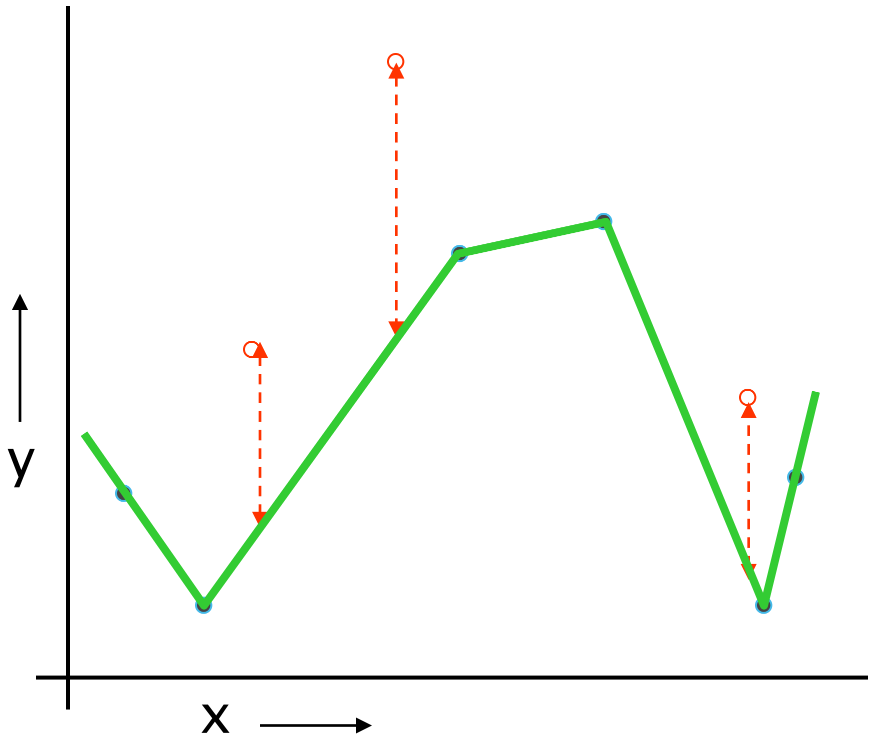
3. Perform your regression on the training set

4. Estimate your future performance with the test set

(Quadratic regression example)

Mean Squared Error = 0.9

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
4. Estimate your future performance with the test set

(Join the dots example)

Mean Squared Error = 2.2

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?

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"

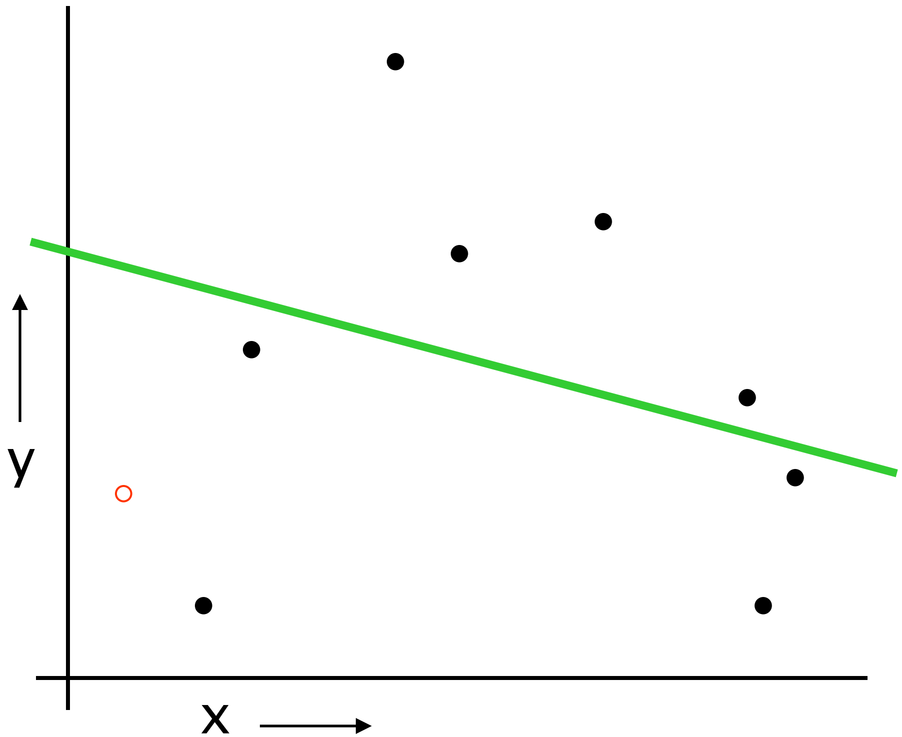
N-Fold Cross Validation

- Popular testing methodology
- Divide data into N even-sized random folds
- For n = 1 to N
  - Train set = all folds except n
  - Test set = fold n
  - Create learner with train set
  - Count number of errors on test set
- Accumulate number of errors across N test sets and divide by N (result is error rate)
- For comparing algorithms, use the same set of folds to create learners (results are paired)

N-Fold Cross Validation

- Advantages/disadvantages
  - Estimate of error within a single data set
  - Every point used once as a test point
  - At the extreme (when N = size of data set), called leave-one-out testing

LOOCV (Leave-one-out Cross Validation)

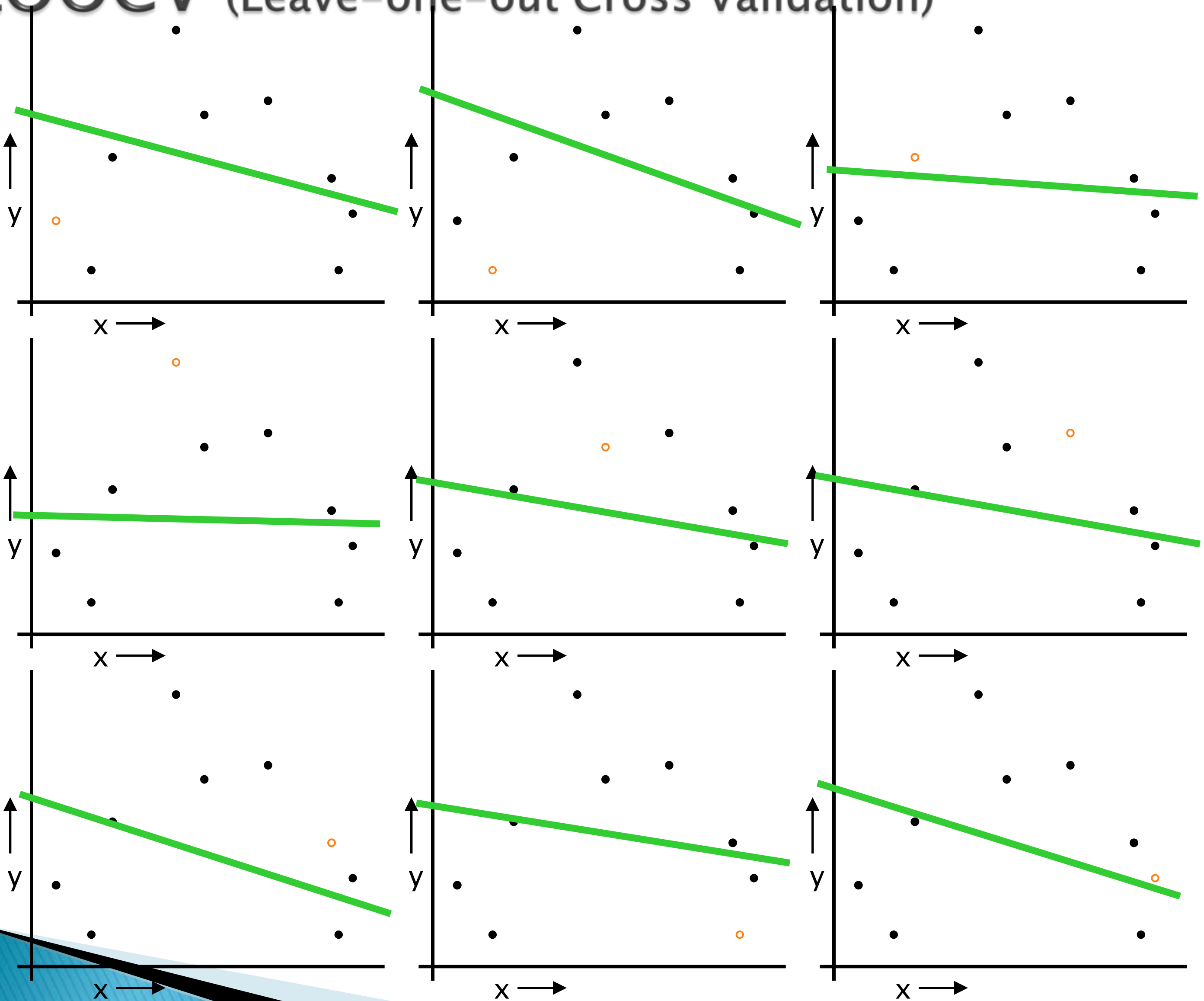


For k=1 to N

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

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

LOOCV (Leave-one-out Cross Validation)



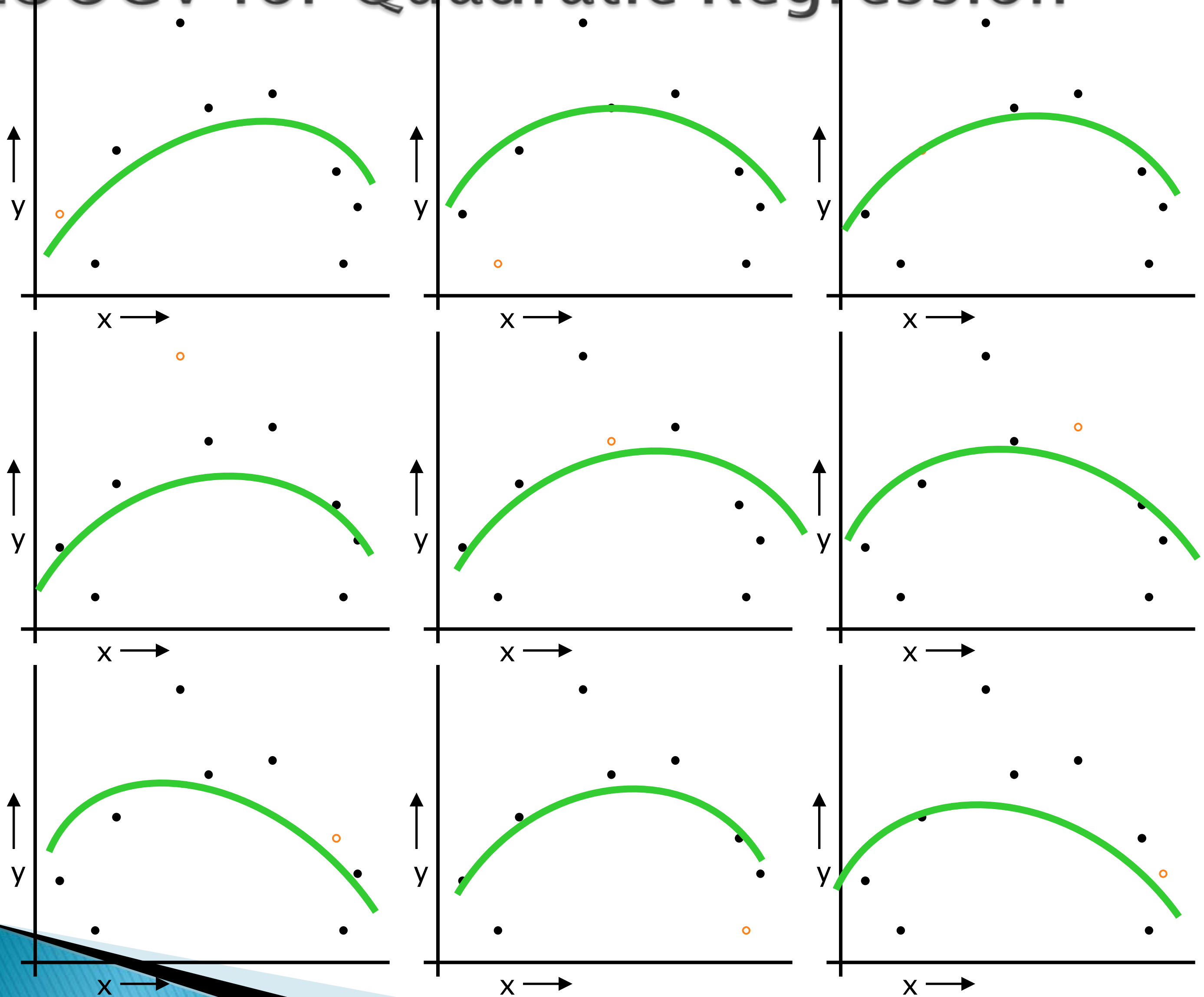
For k=1 to R

1. Let (x_k,y_k) be the k^{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.

$MSE_{LOOCV} = 2.12$

LOOCV for Quadratic Regression



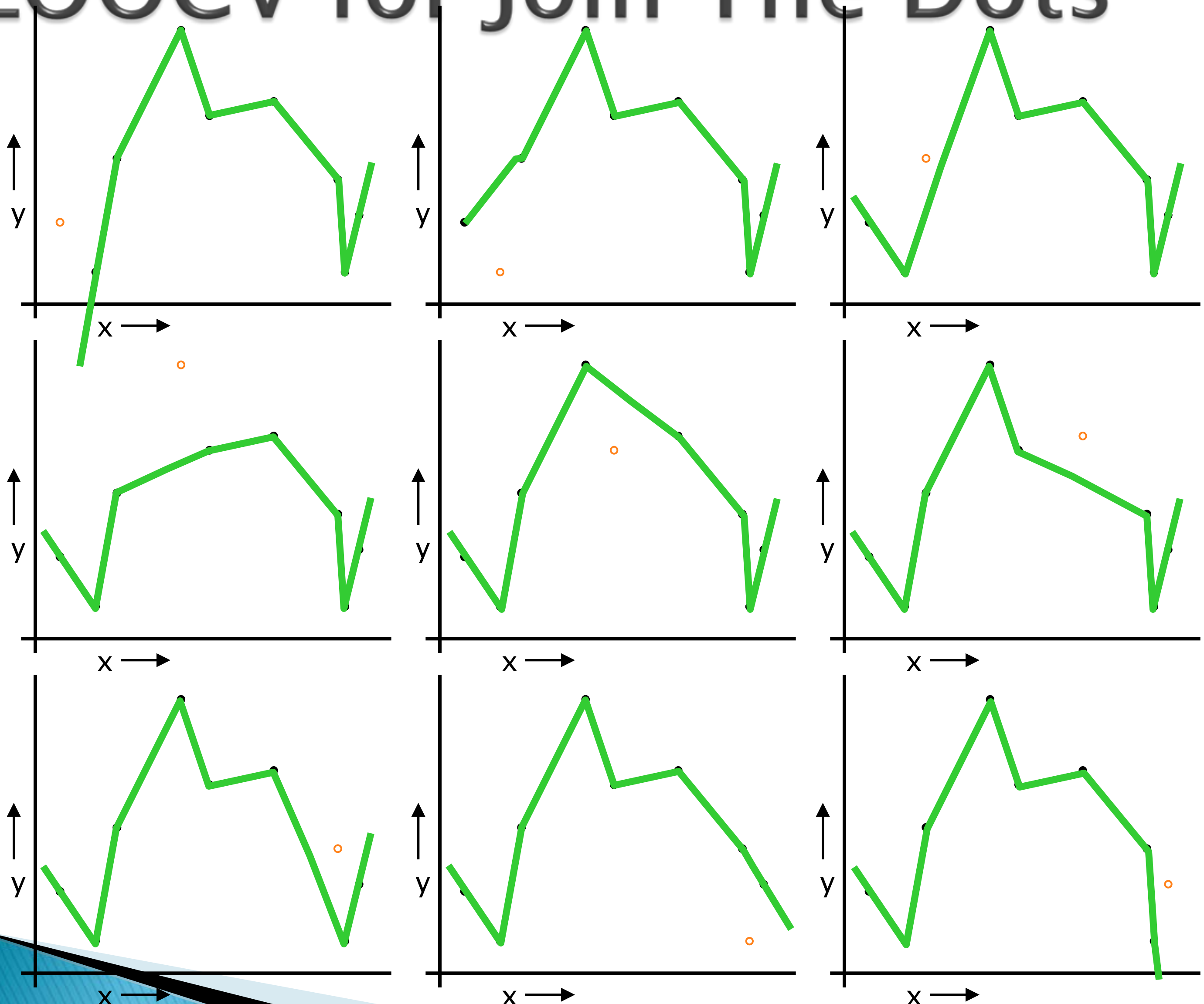
For k=1 to R

1. Let (x_k,y_k) be the k^{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.

$MSE_{LOOCV} = 0.962$

LOOCV for Join The Dots



For k=1 to R

1. Let (x_k,y_k) be the k^{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.

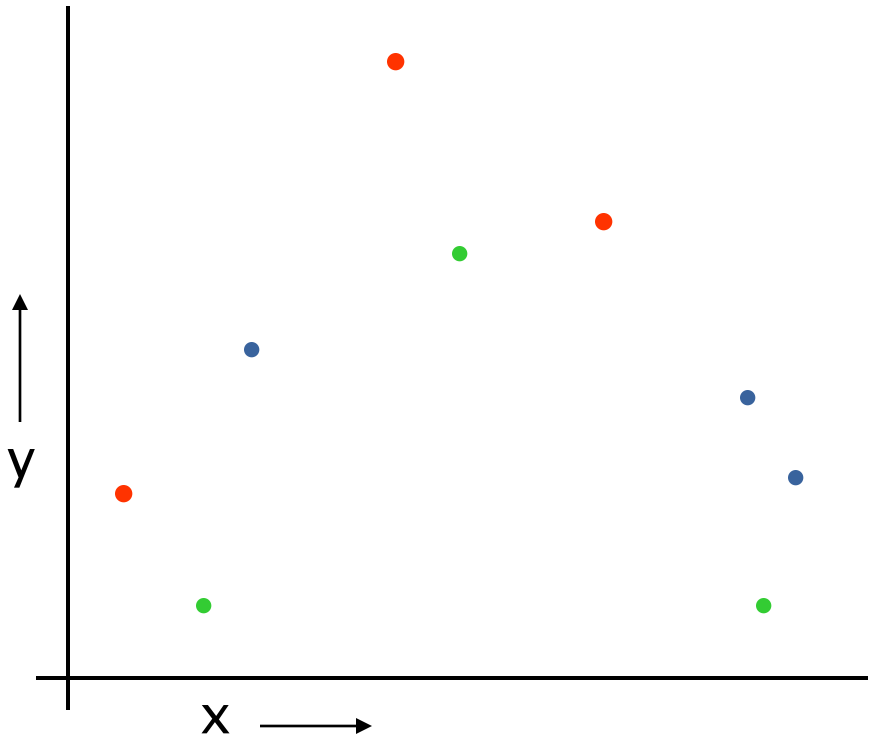
$MSE_{LOOCV} = 3.33$

Which kind of Cross Validation?

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

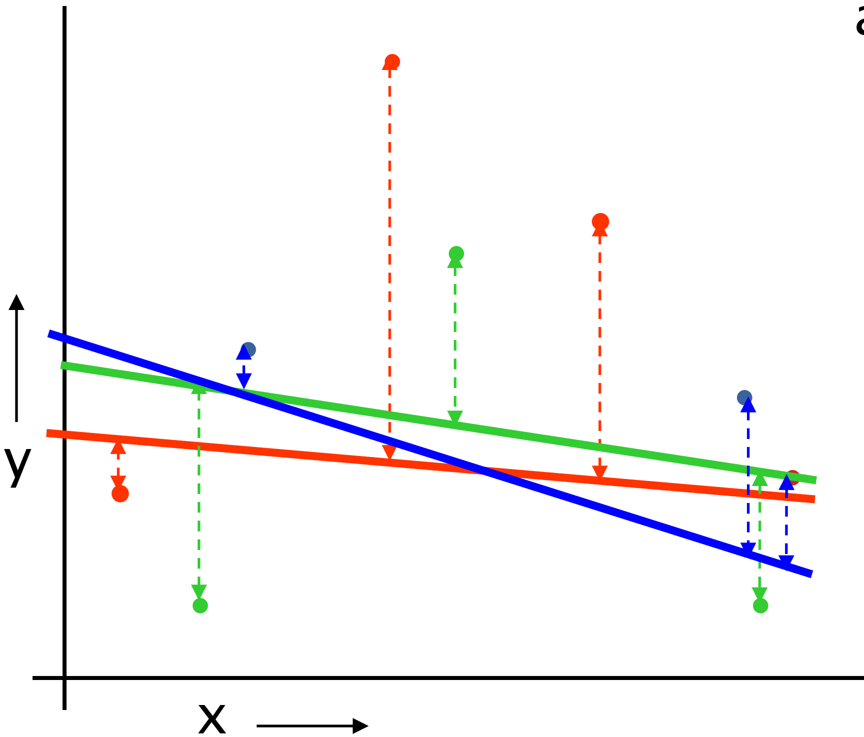
..can we get the best of both worlds?

k-fold CV



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

k-fold CV



Linear Regression

$MSE_{3FOLD}=2.05$

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

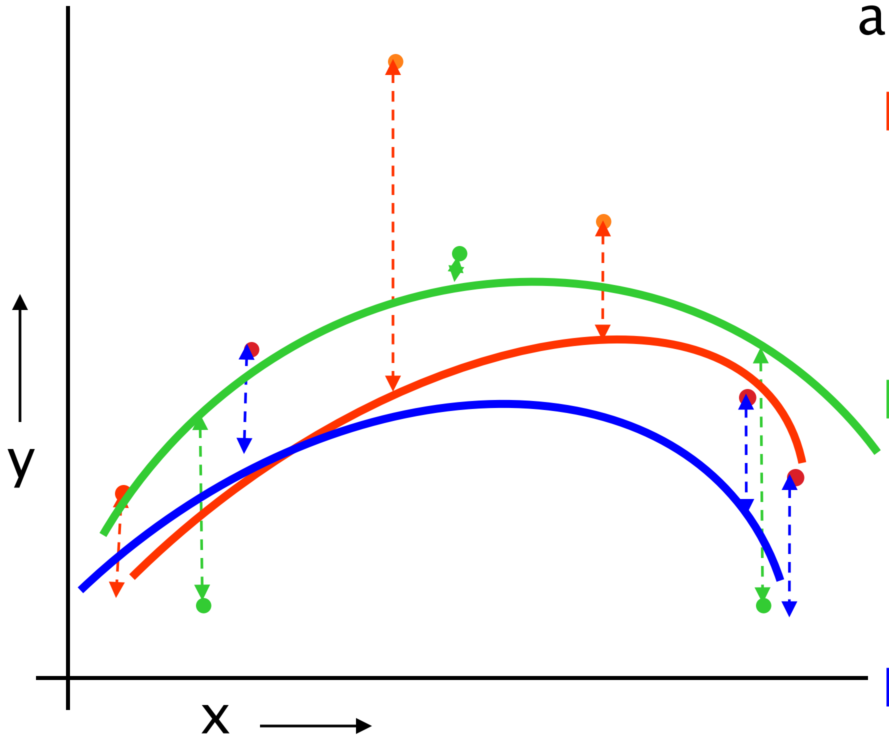
For the red partition: Train on all the points not in the red partition. Find the test-set sum of errors on the red points.

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

Then report the mean error

k-fold CV



Quadratic Regression

$MSE_{3FOLD}=1.11$

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

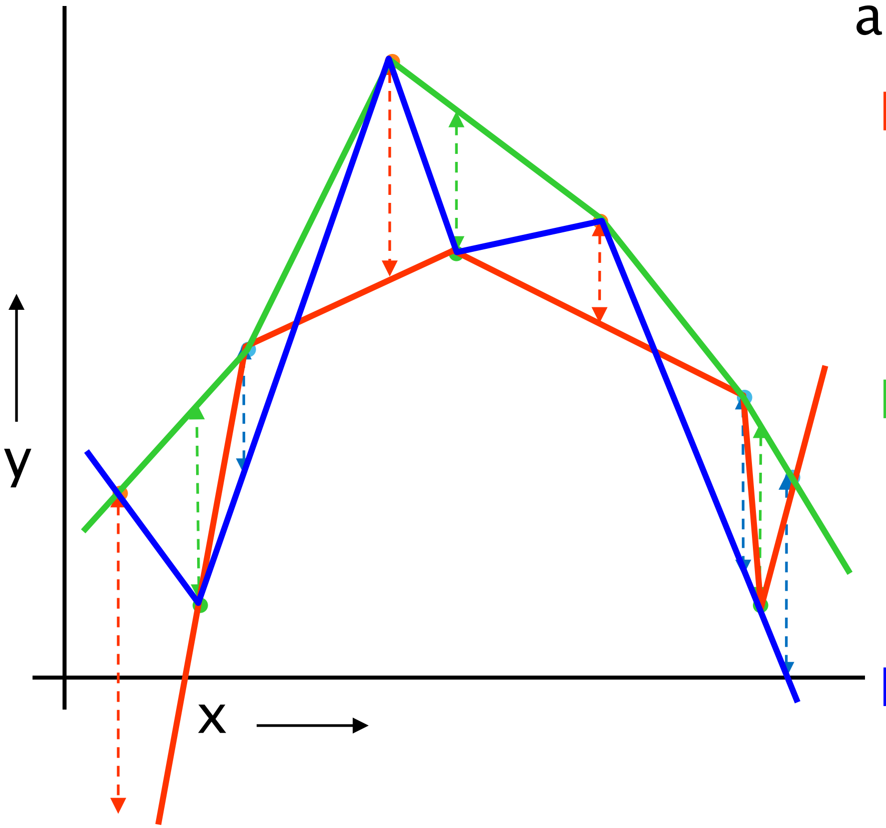
For the red partition: Train on all the points not in the red partition. Find the test-set sum of errors on the red points.

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

Then report the mean error

k-fold CV



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

Then report the mean error

Which kind of Cross Validation?

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

Two Definitions of Error

The **true error** of hypothesis *h* with respect to target function *f* and distribution *D* is the probability that *h* will misclassify an instance drawn at random according to *D*.

$$error_D(h) \equiv \Pr_{x \in D}\left[f(x) \neq h(x)\right]$$

The **sample error** of *h* with respect to target function *f* and data sample *S* is the proportion of examples *h* misclassifies

$$error_S(h) \equiv \frac{1}{n} \sum_{x \in S} \delta\left(f(x) \neq h(x)\right)$$

where $\delta\left(f(x) \neq h(x)\right)$ is 1 if $f(x) \neq h(x)$, and 0 otherwise

How well does $error_S(h)$ estimate $error_D(h)$?

Problems Estimating Error

1. *Bias*: If S is training set, $error_S(h)$ is optimistically biased

$$bias \equiv E[error_S(h)] - error_D(h)$$

For unbiased estimate, h and S must be chosen independently

2. *Variance*: Even with unbiased S, $error_S(h)$ may still vary from $error_D(h)$

Example

Hypothesis *h* misclassifies 12 of 40 examples in *S*.

$$error_S(h) = \frac{12}{40} = .30$$

What is $error_D(h)$?

Estimators

Experiment:

1. Choose sample *S* of size *n* according to distribution *D*
2. Measure $error_S(h)$

   $error_S(h)$ is a random variable (i.e., result of an experiment)

   $error_S(h)$ is an unbiased estimator for $error_D(h)$

Given observed $error_S(h)$ what can we conclude about $error_D(h)$?

Confidence Intervals

If S contains n examples, $n \geq 30$, drawn independently of *h* and each other

Then with approximately N% probability, $error_D(h)$ lies in interval

$$error_S(h) \pm z_N \sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

where

N% :	50%	68%	80%	90%	95%	98%	99%
z_N :	0.67	1.00	1.28	1.64	1.96	2.33	2.53

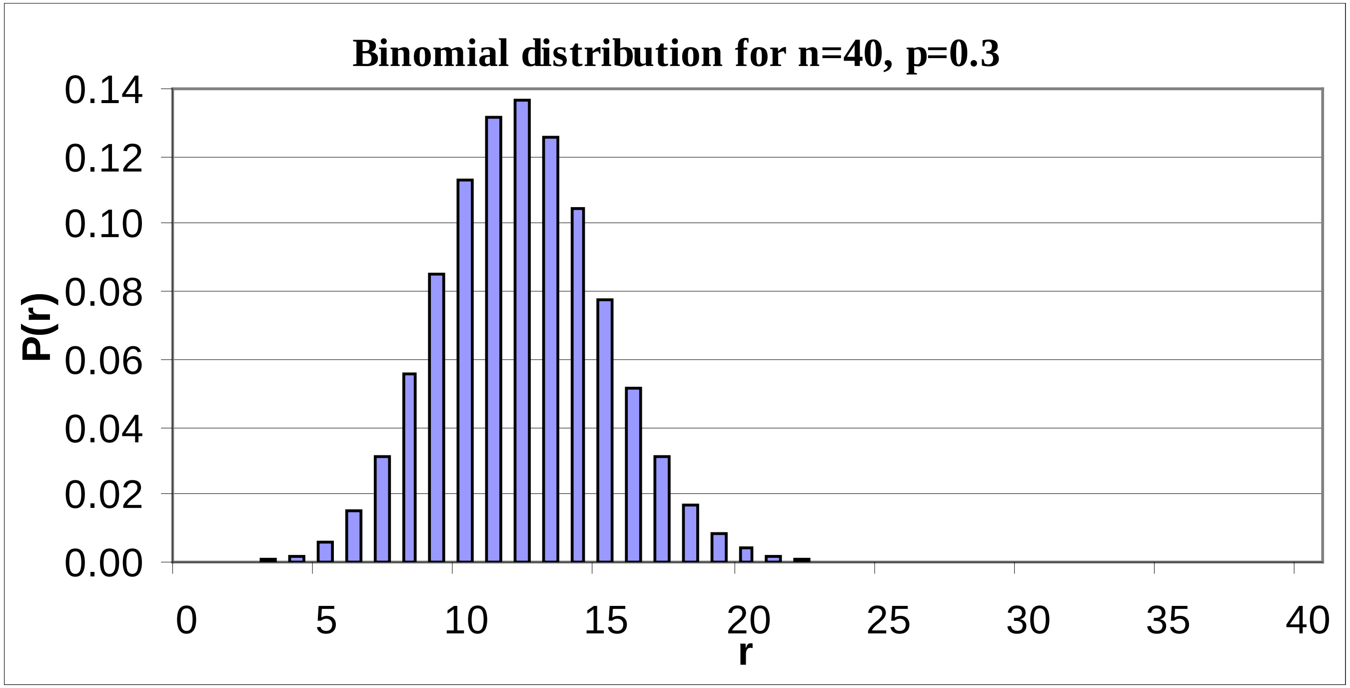
Confidence Intervals

If S contains n examples, drawn independently of h and each other

Then with approximately 95% probability, $error_D(h)$ lies in interval

$$error_S(h) \pm \mathbf{1.96}\sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

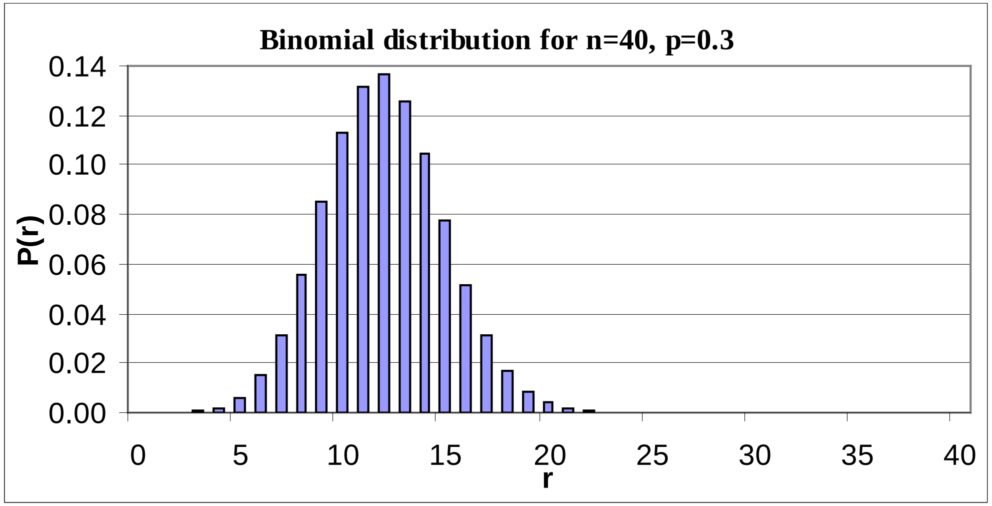
$error_S(h)$ is a Random Variable



- Rerun experiment with different randomly drawn *S* (size *n*)
- Probability of observing *r* misclassified examples:

$$P(r) = \frac{n!}{r!(n-r)!} error_D(h)^r (1 - error_D(h))^{n-r}$$

Binomial Probability Distribution

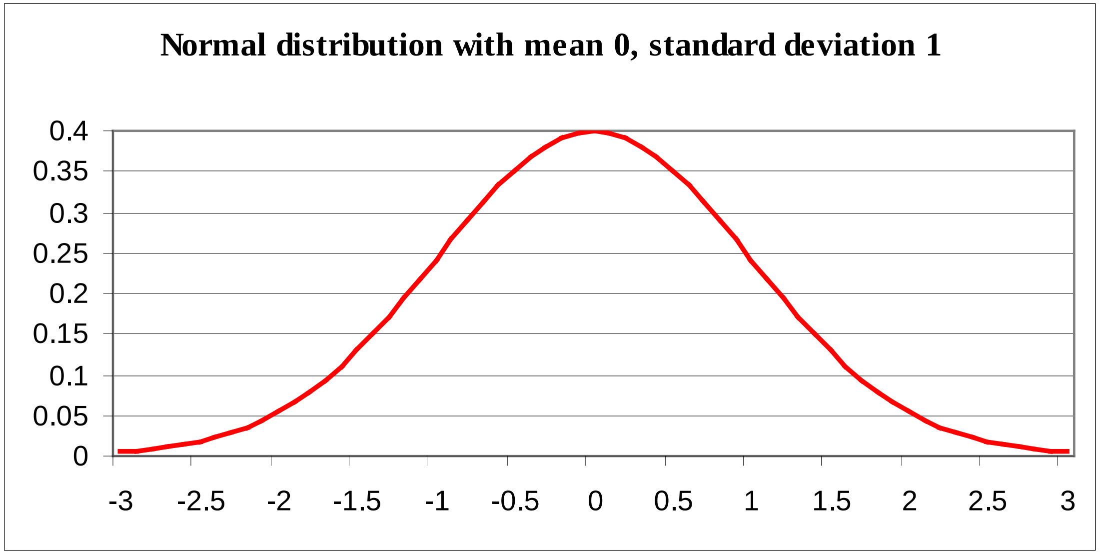


$$P(r) = \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r}$$

Probabilty $P(r)$ of r heads in n coin flips, if $p = \Pr(heads)$

- Expected, or mean value of X : $E[X] \equiv \sum_{i=0}^{n} iP(i) = np$
- Variance of X : $Var(X) \equiv E[(X - E[X])^2] = np(1-p)$
- Standard deviation of X : $\sigma_X \equiv \sqrt{E[(X - E[X])^2]} = \sqrt{np(1-p)}$

Normal Probability Distribution



$$P(r) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

The probability that X will fall into the interval (a,b) is given by

$$\int_a^b p(x)dx$$

- Expected, or mean value of X : $E[X] = \mu$
- Variance of X : $Var(X) = \sigma^2$
- Standard deviation of X : $\sigma_X = \sigma$

Normal Distribution Approximates Binomial

$error_s(h)$ follows a Binomial distribution, with

- mean $\mu_{error_S(h)} = error_D(h)$
- standard deviation

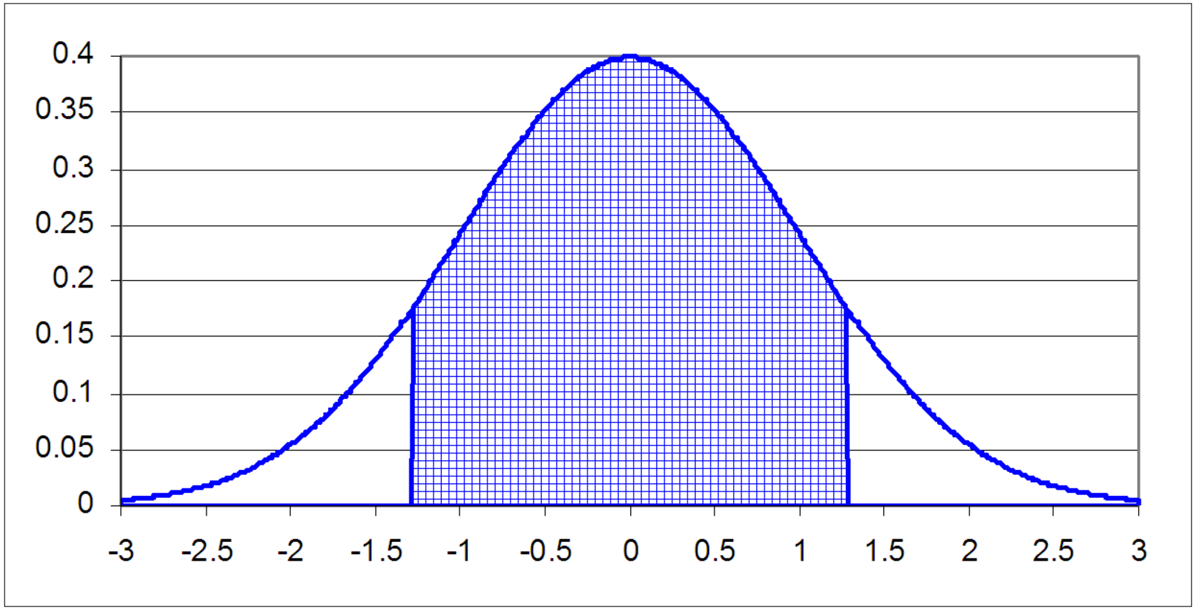
$$\sigma_{error_S(h)} = \sqrt{\frac{error_D(h)(1-error_D(h))}{n}}$$

Approximate this by a Normal distribution with

- mean $\mu_{error_S(h)} = error_D(h)$
- standard deviation

$$\sigma_{error_S(h)} \approx \sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

Normal Probability Distribution



80% of area (probability) lies in $\mu \pm 1.28\sigma$

N% of area (probability) lies in $\mu \pm z_N\sigma$

N% :	50%	68%	80%	90%	95%	98%	99%
z_N :	0.67	1.00	1.28	1.64	1.96	2.33	2.53

Confidence Intervals, More Precisely

If S contains n examples, drawn independently of h and each other $n \geq 30$

Then with approximately 95% probability, *$error_S(h)$* lies in interval

$$error_D(h) \pm 1.96\sqrt{\frac{error_D(h)(1-error_D(h))}{n}}$$

equivalently, *$error_D(h)$* lies in interval

$$error_S(h) \pm 1.96\sqrt{\frac{error_D(h)(1-error_D(h))}{n}}$$

which is approximately

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

Calculating Confidence Intervals

1. Pick parameter p to estimate $error_D(h)$

2. Choose an estimator $error_S(h)$

3. Determine probability distribution that governs estimator

   $error_S(h)$ governed by Binomial distribution, approximated by Normal when $n \geq 30$

4. Find interval (L,U) such that N% of probability mass falls in the interval

   Use table of z_N values

Central Limit Theorem

Consider a set of independent, identically distributed random variables $Y_1 \ldots Y_n$, all governed by an arbitrary probability distribution with mean μ and finite variance σ^2. Define the sample mean

$$\bar{Y} \equiv \frac{1}{n}\sum_{i=1}^{n} Y_i$$

Central Limit Theorem. As $n \to \infty$, the distribution governing $\bar{Y}$ approaches a Normal distribution, with mean μ and variance $\frac{\sigma^2}{n}$.

Difference Between Hypotheses

Test h_1 on sample S_1, test h_2 on S_2

1. Pick parameter to estimate

   $$d \equiv error_D(h_1) - error_D(h_2)$$

2. Choose an estimator

   $$d \equiv error_{S_1}(h_1) - error_{S_2}(h_2)$$

3. Determine probability distribution that governs estimator

   $$\sigma_d \approx \sqrt{\frac{error_{S_1}(h_1)(1 - error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1 - error_{S_2}(h_2))}{n_2}}$$

4. Find interval (L, U) such that N% of probability mass falls in the interval

   $$\hat{d} \pm z_N \sqrt{\frac{error_{S_1}(h_1)(1 - error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1 - error_{S_2}(h_2))}{n_2}}$$

Paired *t* test to Compare L_A, L_B

1. Partition data into k disjoint test sets $T_1, T_2, \ldots, T_k$ of equal size, where this size is at least 30.
2. For i from 1 to k do

   $S_i = \{D - T_i\}$

   $h_A = L_A(S_i)$

   $h_B = L_B(S_i)$

   $\delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$
3. Return the value d, where

$$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$$

N% confidence interval estimate for d :

$$\bar{\delta} \pm t_{N,k-1} s_{\bar{\delta}}$$

$$s_{\bar{\delta}} \equiv \sqrt{\frac{1}{k(k-1)} \sum_{i=1}^{k} (\delta_i - \bar{\delta})^2}$$

Note δ_i approximately Normally distributed

CV for Model selection

- **Training data set** – the set of data used to learn a model or hypothesis
- **Test data set** – the set of data used to estimate some value (often accuracy) related to a model
- **Validation set** – a set of data used to select parameters for a model, often as follows
  - Divide training data into a “sub” training set and validation set
  - For each possible set of parameters
    - Create a model using the “sub” training set
    - Evaluate the model on the validation set and pick the one that performs the best

Bias-Variance Tradeoff: Intuition 1

- The goal in learning is not to learn an exact representation of the training data itself, but to build a statistical model of the process which generates the data. This is important if the algorithm is to have good generalization performance
- We saw that
  - models with too few parameters can perform poorly
  - models with too many parameters can perform poorly
- Need to optimize the complexity of the model to achieve the best performance
- One way to get insight into this tradeoff is the decomposition of generalization error into $\text{bias}^2 + \text{variance}$
  - a model which is too simple, or too inflexible, will have a large bias
  - a model which has too much flexibility will have high variance

Intuition

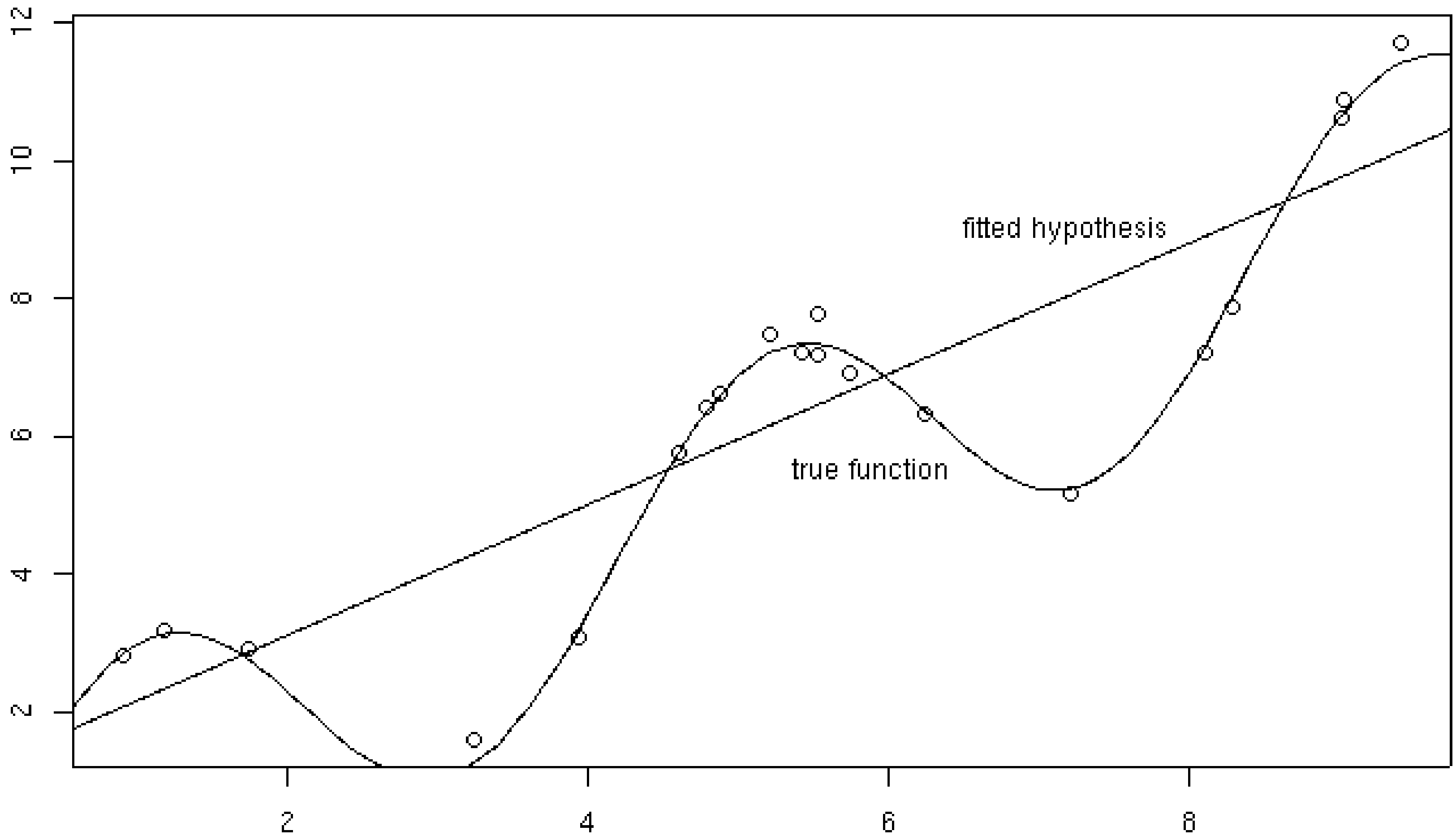
- bias:
  - measures the accuracy or quality of the algorithm
  - high bias means a poor match
- variance:
  - measures the precision or specificity of the match
  - a high variance means a weak match
- We would like to minimize each of these
- Unfortunately, we can’t do this independently, there is a trade-off

Bias-Variance Analysis in Regression

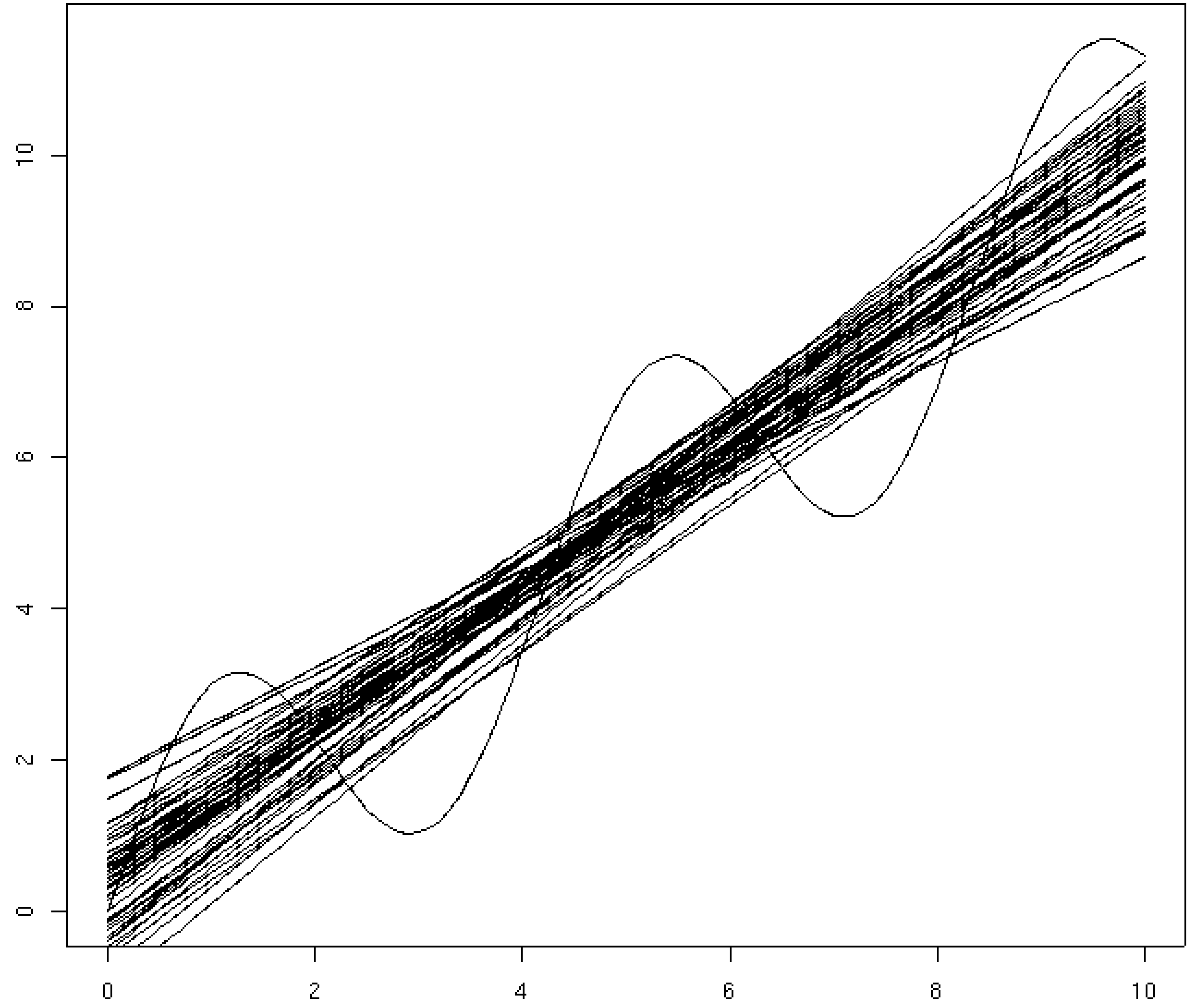
- True function is $y = f(x) + \varepsilon$
  - where ε is normally distributed with zero mean and standard deviation σ.
- Given a set of training examples, $\{(x_i, y_i)\}$, we fit an hypothesis $h(x) = w \cdot x + b$ to the data to minimize the squared error

$$\Sigma_i \, [y_i - h(x_i)]^2$$

Example: 20 points
$y = x + 2 \sin(1.5x) + N(0,0.2)$



50 fits (20 examples each)



Bias-Variance Analysis

- Now, given a new data point x* (with observed value $y^* = f(x^*) + \varepsilon$, we would like to understand the expected prediction error

$$E[\,(y^* - h(x^*))^2\,]$$

Classical Statistical Analysis

- Imagine that our particular training sample S is drawn from some population of possible training samples according to P(S).
- Compute E_P [$(y^* - h(x^*))^2$]
- Decompose this into “bias”, “variance”, and “noise”

Lemma

- Let Z be a random variable with probability distribution P(Z)
- Let $\overline{Z} = E_P[\ Z\ ]$ be the average value of Z.
- Lemma : $E[\ (Z - \overline{Z})^2\ ] = E[Z^2] - \overline{Z}^2$

$$E[\ (Z - \overline{Z})^2\ ] = E[\ Z^2 - 2\,Z\,\overline{Z} + \overline{Z}^2\ ]$$
$$= E[Z^2] - 2\,E[Z]\,\overline{Z} + \overline{Z}^2$$
$$= E[Z^2] - 2\,\overline{Z}^2 + \overline{Z}^2$$
$$= E[Z^2] - \overline{Z}^2$$

- Corollary : $E[Z^2] = E[\ (Z - \overline{Z})^2\ ] + \overline{Z}^2$

Bias–Variance–Noise Decomposition

$$E[\,(h(x^*) - y^*)^2\,] = E[\,h(x^*)^2 - 2\,h(x^*)\,y^* + y^{*2}\,]$$

$$= E[\,h(x^*)^2] - 2\,E[h(x^*)]E[\,y^*] + E[y^{*2}\,]$$

$$= E[\,\left(h(x^*) - \overline{h(x^*)}\right)^2] - \overline{h(x^*)}^2$$

$$- 2\,\overline{h(x^*)}f(x^*)$$

$$+ E[(y^* - f(x^*))^2\,] + f(x^*)^2$$

$$= E[\,\left(h(x^*) - \overline{h(x^*)}\right)^2] + \qquad \text{VARIANCE}$$

$$\left(\overline{h(x^*)}^2 - f(x^*)\right)^2 \qquad \text{BIAS}$$

$$+ E[(y^* - f(x^*))^2\,] \qquad \text{NOISE}$$

$$= \mathrm{Var}(h(x^*)) + \mathrm{Bias}(h(x^*))^2 + E[\varepsilon^2\,]$$

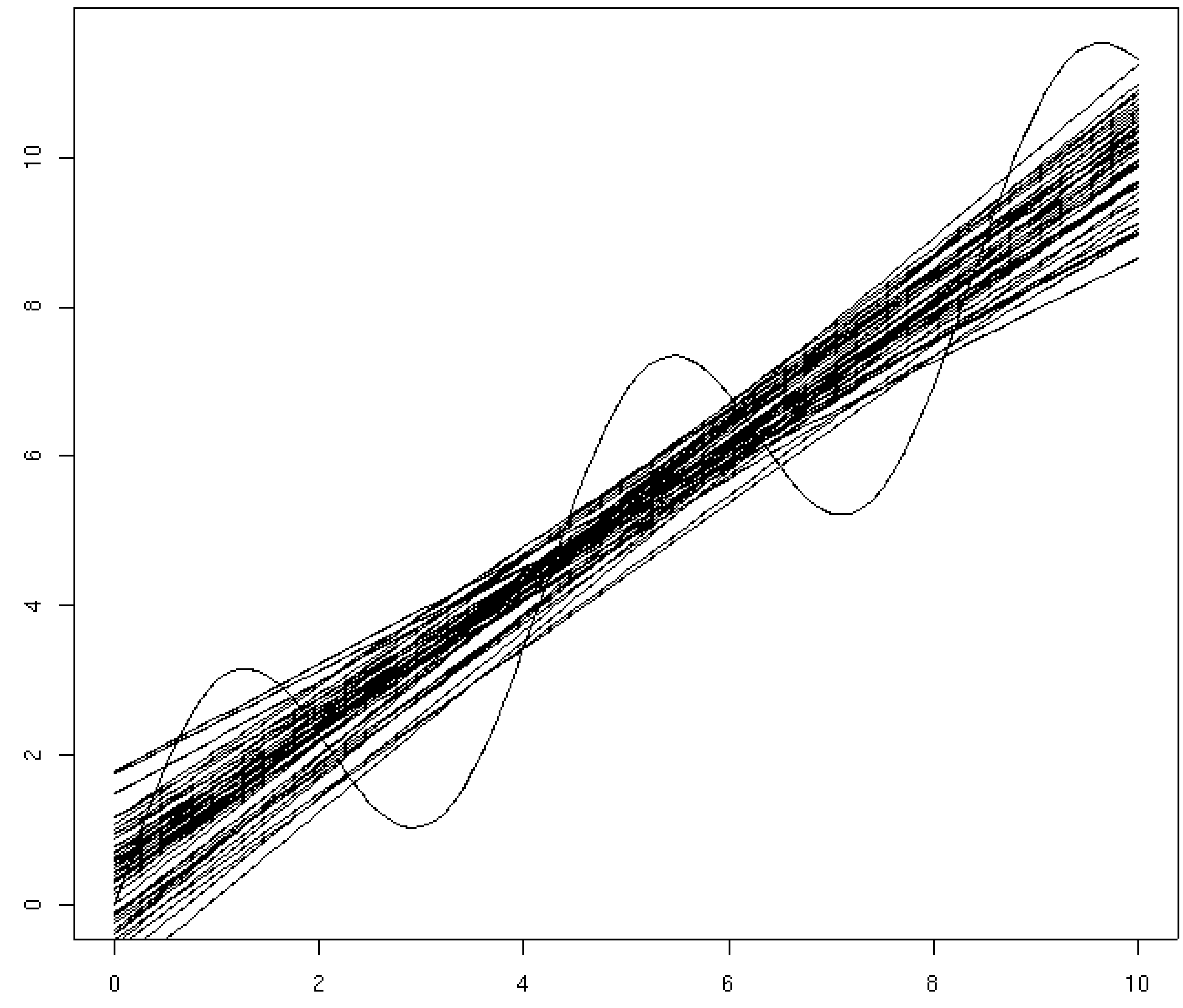
$$= \mathrm{Var}(h(x^*)) + \mathrm{Bias}(h(x^*))^2 + \sigma^2$$

Expected prediction error = Variance + Bias^2 + Noise^2

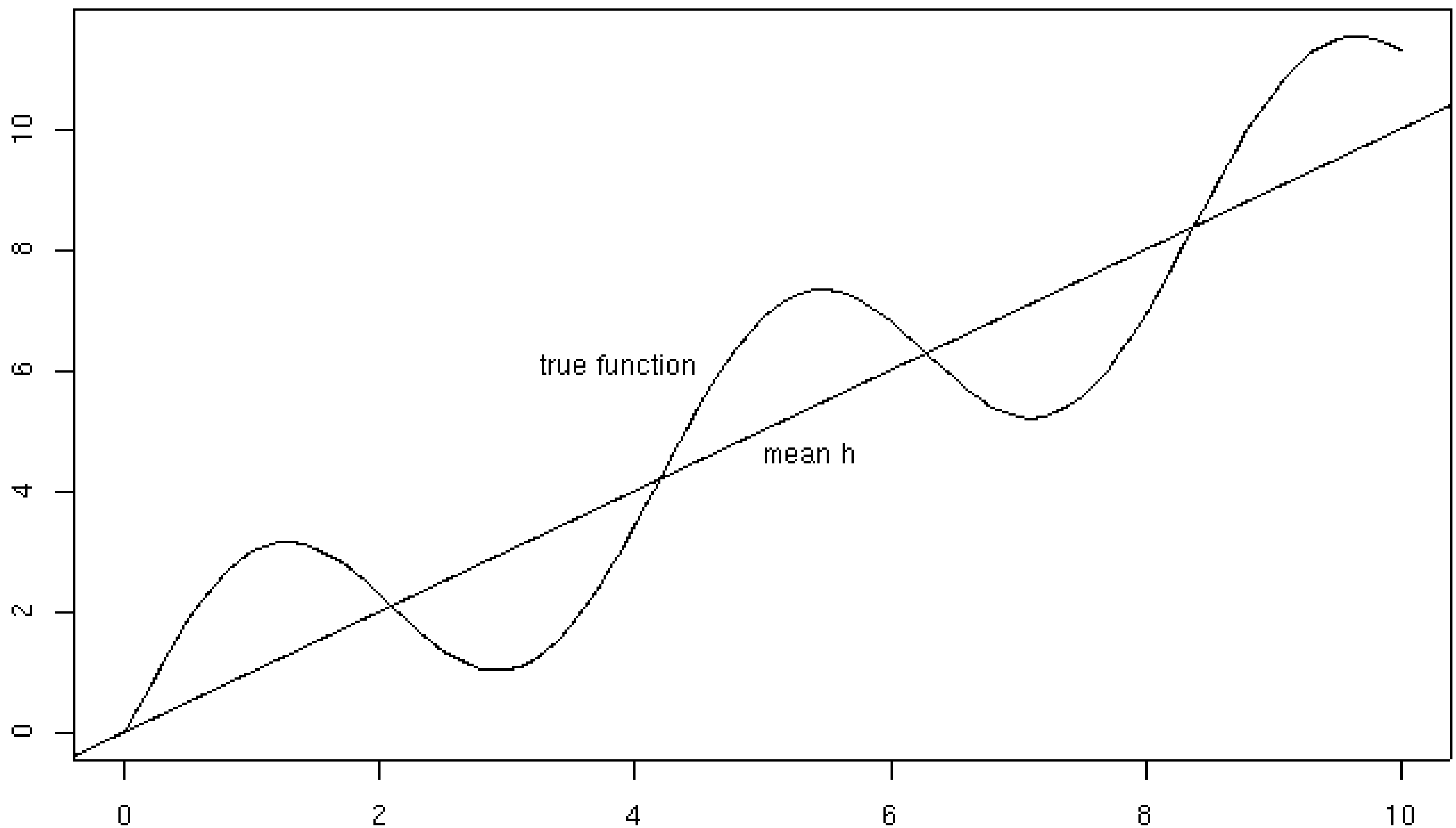
Bias, Variance, and Noise

- Variance: $E[\,(h(x^*) - \bar{h}(x^*))^2\,]$
  Describes how much $h(x^*)$ varies from one training set S to another
- Bias: $[\bar{h}(x^*) - f(x^*)]$
  Describes the average error of $h(x^*)$.
- Noise: $E[\,(y^* - f(x^*))^2\,] = E[\varepsilon^2] = \sigma^2$
  Describes how much y^* varies from $f(x^*)$

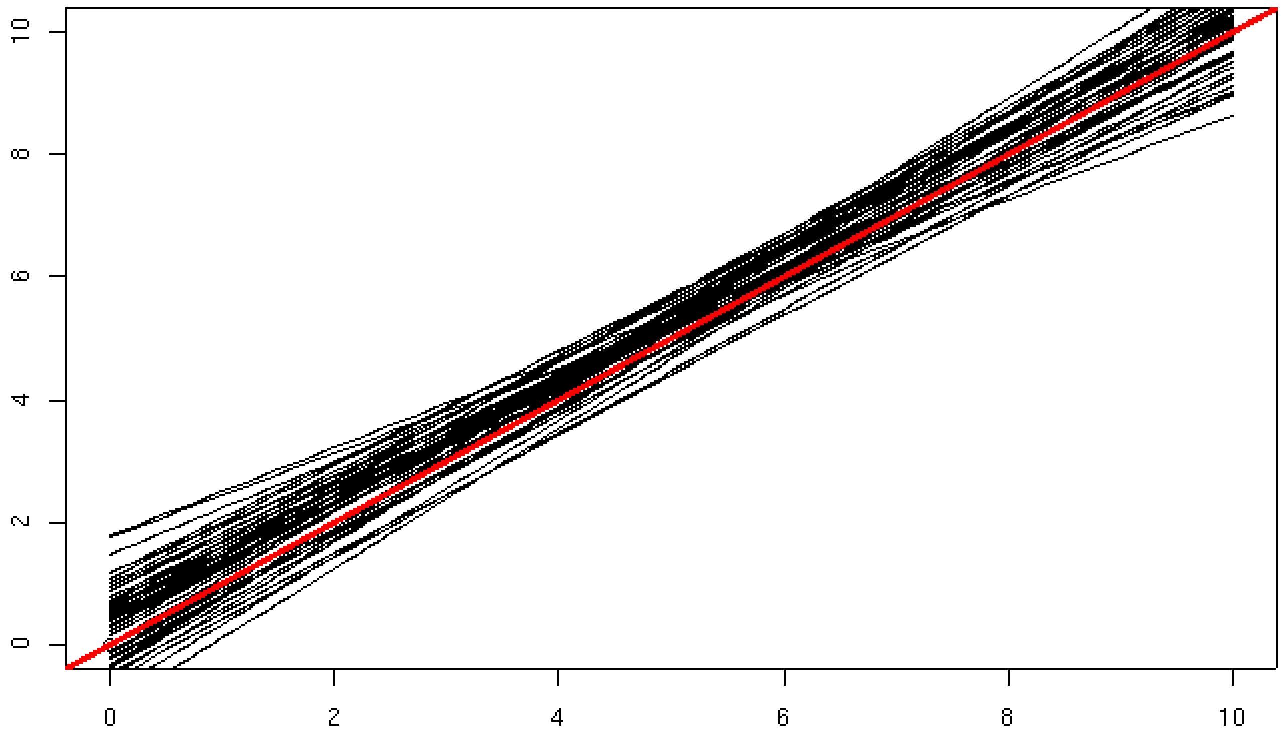
50 fits (20 examples each)



Bias



Variance



Noise