













Inspire...Educate...Transform.

# **Statistics and Probability in Decision Modeling**

Logistic Regression, ROC and AUC, Gains and Lift Charts, Naïve Bayes Classifier, Performance Measures

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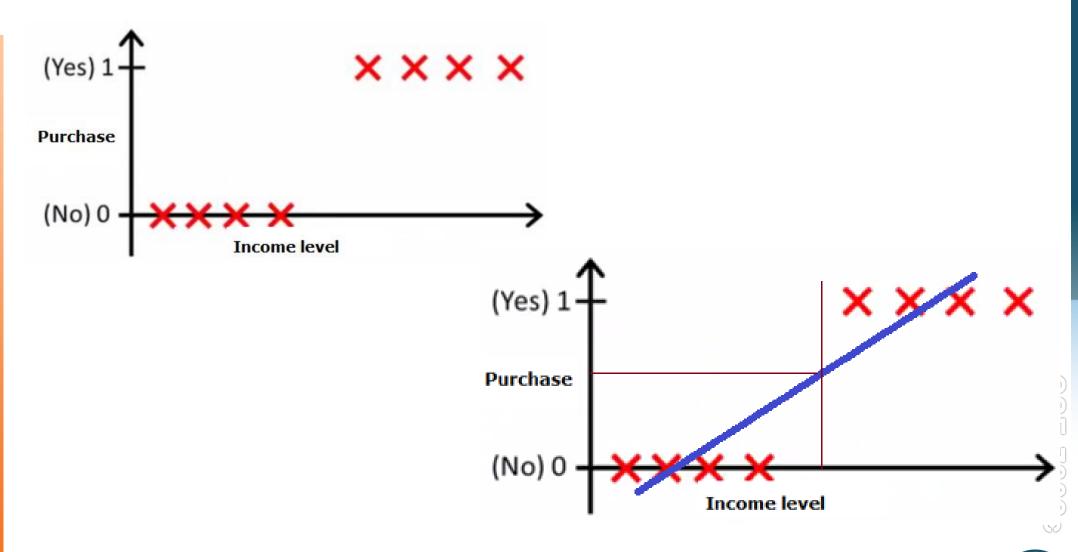
January 07, 2018

### **LOGISTIC REGRESSION**



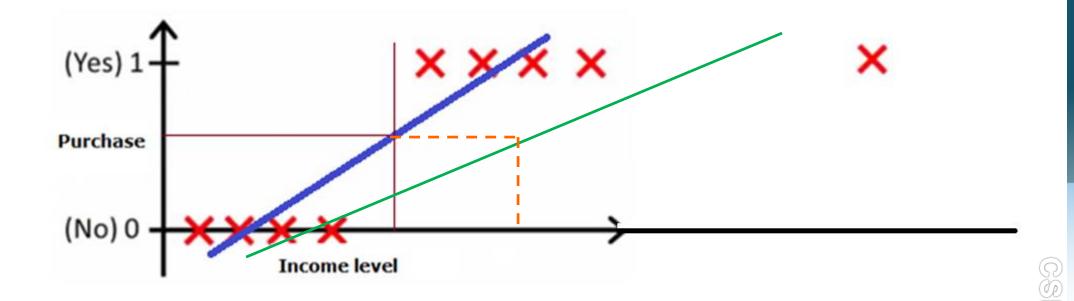


## **Classification Tasks: Regression**





### It could fail



In addition, linear regression hypothesis can be much larger than 1 or much smaller than zero and hence thresholding becomes difficult.





## **No Assumptions**

Ordinary Least Squares (OLS) is inappropriate.

Maximum Likelihood Estimation (MLE) is used instead.

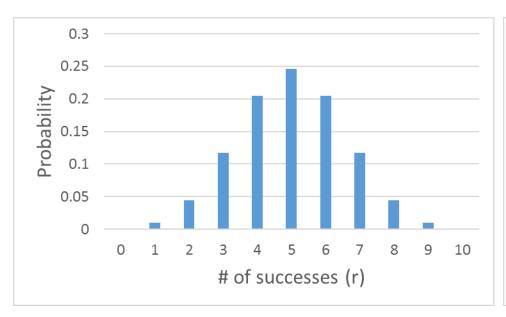
Hence avoids assumptions regarding normality and homoscedasticity of errors, and linearity between dependent and independent variables.

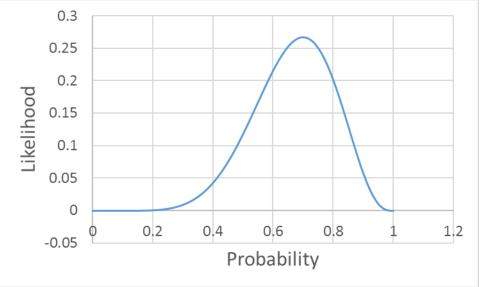




### **Probability vs Likelihood - Excel**

- Likelihood is also known as reverse probability.
- In Probability, we **predict data** based on **known parameters**. (Recall B(n,p), Geo(p),  $Po(\lambda)$ ,  $N(\mu, \sigma^2)$ , etc.)
- In Likelihood, we **predict parameters** based on **known data**.



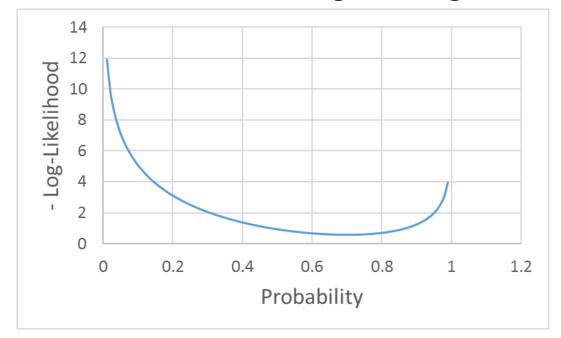




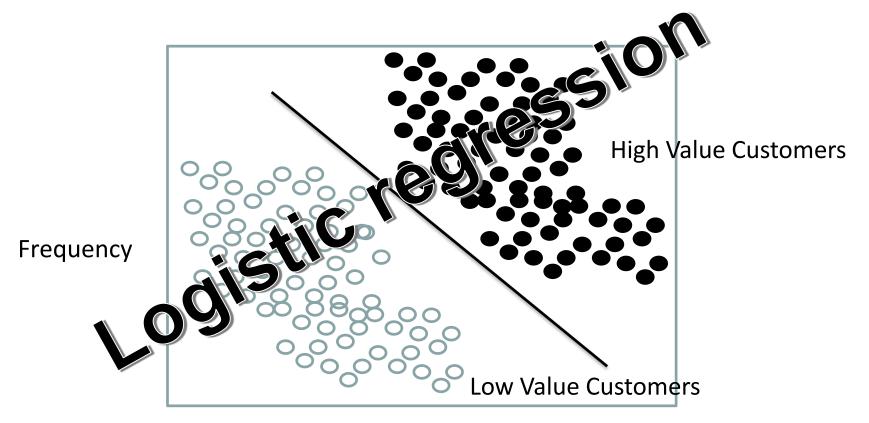


### **MLE**

- Goal is to maximize likelihood.
- In most Data Science optimizations, the goal is to find minima using calculus (minimize sum of squared errors in linear regression, and so on) or numerical techniques like Gradient Descent (minimize deviance in logistic regression, and so on).
- Maximum Likelihood => Minimum of Negative Log-Likelihood.







Transaction value



# **Example**

An auto club mails a flier to its members offering to send more information regarding a supplemental health insurance plan if the member returns a brief enclosed form.

Can a model be built to predict if a member will return the form or not?





# Example

$$f(x) = p = \frac{1}{1 + e^{-\mu}} = \frac{e^{\mu}}{1 + e^{\mu}}$$

where  $\mu = \beta_0 + \beta_1 x_1$  (also known as the systematic or the structural component or linear predictor).

This is a logistic model. The function is also known as the inverse link function, which links the response with the systematic component.

p is the probability that a club member fits into group 1 (returns the form; success; P(Y=1|X)).



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# Logistic model

$$f(x) = p = \frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}}{1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}}$$

Odds Ratio is obtained by the probability of an event occurring divided by the probability that it will not occur.

Logistic model can be transformed into an odds ratio:

$$S = Odds \ ratio = \frac{p}{1 - p}$$





### **Attention Check – Probability and Odds**

If the probability of winning is 6/12, what

1:1 (Note, the probability of

are the odds of winning?

losing also is 6/12)

If the odds of winning are 13:2, what is

13/15

8/11

the probability of winning?

If the odds of winning are 3:8, what is the

probability of losing?

If the probability of losing is 6/8, what

are the odds of winning?

2:6 or 1:3





# Logistic model

$$S = Odds \ ratio = \frac{p}{1 - p}$$

$$S = \frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}}{1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}}$$

$$1 - \frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}}{1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}}$$

$$\therefore S = e^{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}$$

$$\ln(S) = \ln\left(e^{\beta_0 + \beta_1 x_1 + \dots + \beta_k x_k}\right) = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k$$





# Logistic model

The log of the odds ratio is called logit, and the transformed model is linear in  $\beta$ s.







# and Interpreting the output

```
call:
glm(formula = Response ~ Age, family = "binomial", data = flierresponse)
Deviance Residuals:
               1Q Median
    Min
                                   3Q
                                           Max
-1.95015 -0.32016 -0.05335 0.26538 1.72940
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -20.40782 4.52332 -4.512 6.43e-06 ***
                       0.09482 4.492 7.05e-06 ***
             0.42592
Age
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)
    Null deviance: 123.156 on 91 degrees of freedom
Residual deviance: 49.937 on 90 degrees of freedom
AIC: 53.937
Number of Fisher Scoring iterations: 7
```

What is the logit equation?

$$\ln(S) = -20.40782 + 0.42592Age$$





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### **Determining Logistic Regression Model**

Suppose we want a probability that a 50-year old club member will return the form.

$$\ln(S) = -20.40782 + 0.42592 * 50 = 0.89$$
$$S = e^{0.89} = 2.435$$

The odds that a 50-year old returns the form are 2.435 to 1.





### **Determining Logistic Regression Model**

$$\hat{p} = \frac{S}{S+1} = \frac{2.435}{2.435+1} = 0.709$$

Using a probability of 0.50 as a cutoff between predicting a 0 or a 1, this member would be classified as a 1.





### **Interpreting Output - Deviances**

**Deviance** or **Residual Deviance** is *similar to SSE* in the sense it measures how much remains unexplained by the model built with predictors included.

$$D=-2LL$$

where LL is the log-likelihood.

**Null Deviance** shows how well the model predicts the response with only the intercept as a parameter. The intercept is the logarithm of the ratio of cases with y=1 to the number of cases with y=0. This is *similar to SST*, which gives total variation when all coefficients are zero (null hypothesis).



### Interpreting Output – Testing the Overall Model

The z-values and the associated p-values provide significance of individual predictor variables.

R outputs AIC (Akaike's Information Criterion) and you need to pick the model with the lowest AIC.

```
glm(formula = Response ~ Age, family = "binomial", data = flierresponse)
Deviance Residuals:
    Min
                     Median
-1.95015 -0.32016 -0.05335
                              0.26538
                                        1.72940
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -20.40782
                        4.52332 -4.512 6.43e-06 ***
              0.42592
                        0.09482
                                4.492 7.05e-06 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '1
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 123.156 on 91 degrees of freedom
Residual deviance: 49.937 on 90 degrees of freedom
AIC: 53.937
Number of Fisher Scoring iterations: 7
```

http://www.insofe.edu.in





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### Interpreting Output – Testing the Overall Model

- AIC provides a means for model selection.
- AIC = D + 2k, where k is the # of parameters in the model including the intercept. Recall in Linear Regression, it is calculated as AIC = nIn(RSS/n) + 2k.
- AIC is *similar to Adjusted*  $R^2$  in the sense it penalizes for adding more parameters to the model.
- It does not test a model in the sense of null hypothesis and hence doesn't tell anything about the quality of the model. It is only a relative measure between multiple models.



# **Applications**

- Predicting stock price movement (up/down)
- Predict whether a patient has diabetes or not
- Predict whether a customer will buy or not
- Predict the likelihood of loan default





# **Diagnostic Hints**

 Coefficients that tend to infinity could be a sign that an input is perfectly correlated with a subset of your responses. Or put another way, it could be a sign that this input is only really useful on a subset of your data, so perhaps it is time to segment the data.





# **Diagnostic Hints**

- Overly large coefficient magnitudes, overly large error bars on the coefficient estimates, and the wrong sign on a coefficient could be indications of correlated inputs.
- VIF can be used to check for multicollinearity. R outputs a Generalized Variance Inflation Factor, which is obtained by correcting VIF to the degrees of freedom for categorical predictors.  $GVIF = VIF^{\left(\frac{1}{2*df}\right)}$





# **Case – Framingham Heart Study**



- Committed to identifying common factors contributing to cardiovascular disease (CVD).
- Setup in the town of Framingham, MA in 1948.

Random sample consisting of 2/3rds of adult population in the

town.

AGE-SEX DISTRIBUTION AT ENTRY (1948)				
29-39	40-49	50-62	Totals	
835	779	722	2,336	
1,042	962	869	2,873	
1,877	1,741	1,591	5,209	
	<b>29-39</b> 835 1,042	29-39     40-49       835     779       1,042     962	29-39     40-49     50-62       835     779     722       1,042     962     869	





#### Case Study – Data (framinghamheartstudy.org and MITx)

- 5209 men and women participated.
- Age range: 30-62
- People who had not yet developed overt symptoms of CVD or suffered a heart attack or stroke.
- Careful monitoring of Framingham Study population has led to identification of major CVD risk factors.
- Led to development of Framingham Risk Score, a gender specific algorithm used to estimate the 10-year cardiovascular risk of an individual:

http://cvdrisk.nhlbi.nih.gov/





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#### Data description

4240 observations; 15 predictor and 1 predicted variables

 TenYearCHD – To be predicted. Risk of having a heart attack or stroke in the next 10 years.

#### **Predictors**

- Demographic Risk Factors
  - male: Gender of subject Yes or No
  - age: Age of subject at first examination
  - education: some high school (1), high school (2), some college/vocational college (3), college (4)





- Behavioural Risk Factors
  - currentSmoker: Yes or No
  - cigsPerDay: No. of cigarettes smoked per day if smoker
- Medical History Risk Factors
  - BPmeds: On BP medication at the time of first examination Yes or No
  - prevalentStroke: Did the subject have a previous stroke Yes or No
  - prevalentHyp: Is the subject currently hypertensive Yes or No
  - diabetes: Does the subject currently have diabetes Yes or No





- Risk Factors from First Examination
  - totChol: Total cholesterol (mg/dL)
  - sysBP: Systolic blood pressure (the higher number in BP result)
  - diaBP: Diastolic blood pressure (the lower number in BP result)
  - BMI: Body Mass Index (kg/m²)
  - heartRate: # of beats per minute
  - glucose: Blood glucose level (mg/dL)





### Approach

- Randomly split data into training and test in 70:30 ratio.
- Measure prediction accuracies on training and test data





#### Results

- Significant variables that cannot be controlled
  - Gender
  - Age
  - Medical history
- Significant variables that can be controlled
  - Smoking habits
  - Cholesterol
  - Systolic BP
  - Blood glucose

```
call:
glm(formula = TenYearCHD ~ ., family = binomial, data = train)
Deviance Residuals:
    Min
                   Median
                                        Max
-1.9392 -0.5998 -0.4211 -0.2771
                                     2.8632
Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
(Intercept)
                            0.864696 -9.668 < 2e-16 ***
                -8.360272
                            0.130836
male
                 0.524080
                 0.065429
                            0.008049
age
                                       8.129 4.34e-16 ***
education
                -0.041105
                            0.059185 -0.695 0.487366
currentSmoker
                            0.187629
                 0.120498
                                       0.642 0.520735
cigsPerDay
                 0.016471
                            0.007488
                                       2.200 0.027825 *
BPMeds
                 0.169118
                            0.282140
                                       0.599 0.548898
prevalentStroke 1.156666
                            0.560179
                                       2.065 0.038940 *
prevalentHyp
                            0.166034
                 0.307077
                                       1.849 0.064389 .
                            0.392574
diabetes
                -0.319937
                                      -0.815 0.415087
totChol
                 0.003799
                            0.001330
                                       2.856 0.004290 **
                 0.011144
                            0.004446
                                       2.507 0.012188 *
SysBP
diaBP
                -0.001861
                            0.007760 -0.240 0.810517
                 0.008812
                            0.015662
                                       0.563 0.573702
                -0.007273
                            0.005131 -1.418 0.156296
heartRate
glucose
                 0.009227
                            0.002752
                                       3.353 0.000798 ***
                0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Signif. codes:
(Dispersion parameter for binomial family taken to be 1)
    Null deviance: 2176.6 on 2565 degrees of freedom
Residual deviance: 1919.9 on 2550 degrees of freedom
  (402 observations deleted due to missingness)
AIC: 1951.9
```



#### Results

- Accuracy in training set = 2200/2566 = 85.7%
- Accuracy in testing set = 927/1092 = 84.9%

- Accuracy is affected by imbalance between positives and negatives.
- There is a trade-off between sensitivity and specificity.

#### **Training Set**

10-year CHD risk		Predicted		
		True	False	
Actual	True	30	357	
	False	9	2170	

#### **Testing Set**

10-year CHD risk		Predicted		
		True	False	
Actual	True	12	158	
	False	7	915	







# Some More Performance Measures for Regression and Classification Models





### **ROC Curves and AUC**

- ROC Receiver Operating Characteristics
- AUC Area Under the ROC Curve







### **ROC Curves and AUC**

 ROC – Plot of True Positive Rate vs False Positive Rate, i.e., Sensitivity vs 1-Specificity

Probability Threshold for Discriminating Between High Risk and Low Risk of Having Ten Year CHD	True Positives	False Positives	True Negatives	False Negatives
0.9	0	0	922	170
0.7	1	1	921	169
0.5	12	7	915	158
0.3	46	76	846	124
0.1	140	468	454	30

Actual Counts

- Without CHD: 922

With CHD: 170



### **ROC Curves and AUC**

ROC – Plot of True Positive Rate vs False Positive Rate, i.e., Sensitivity

vs 1-Specificity

	Sensitivity		Specificity	
Probability Threshold for Discriminating Between High Risk and Low Risk of Having Ten Year CHD	True Positive Rate	False Positive Rate	True Negative Rate	False Negative Rate
0.9	0/170	0/922	922/922	170/170
0.7	1/170	1/922	921/922	169/170
0.5	12/170	7/922	915/922	158/170
0.3	46/170	76/922	846/922	124/170
0.1	140/170	468/922	454/922	30/170



- Without CHD: 922

With CHD: 170

**ROC Curve** 

C -- - -: f: -: +.





ROC – Plot of True Positive Rate vs False Positive Rate, i.e., Sensitivity

Sancitivity

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vs 1-Specificity

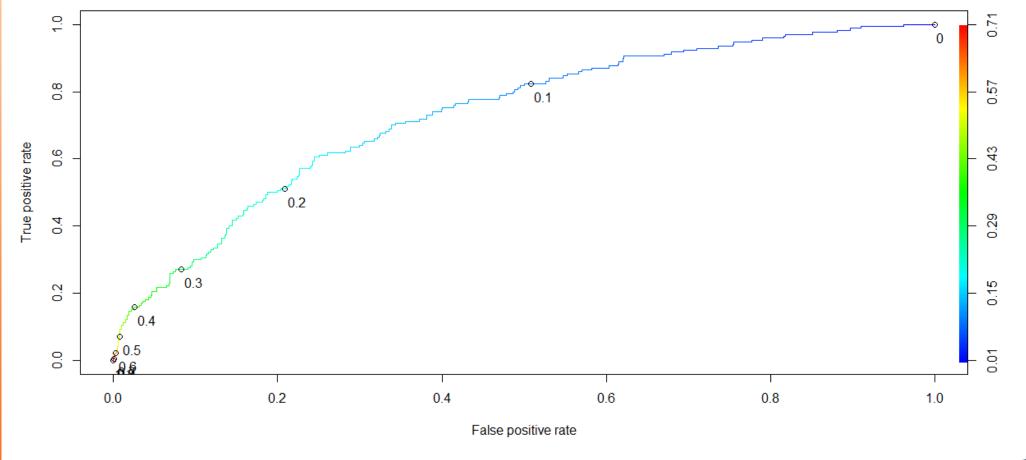
	Selisitivity		
Probability Threshold for Discriminating Between High Risk and Low Risk of Having Ten Year CHD	True Positive Rate	False Positive Rate	
0.9	0/170	0/922	
0.7	1/170	1/922	ROC Curve
0.5	12/170	7/922	
0.3	46/170	76/922	
0.1	140/170	468/922	
		1	

P(Predicting CHD | Have CHD)

P(Predicting CHD | Do Not Have CHD)



 ROC – Plot of True Positive Rate vs False Positive Rate, i.e., Sensitivity vs 1-Specificity

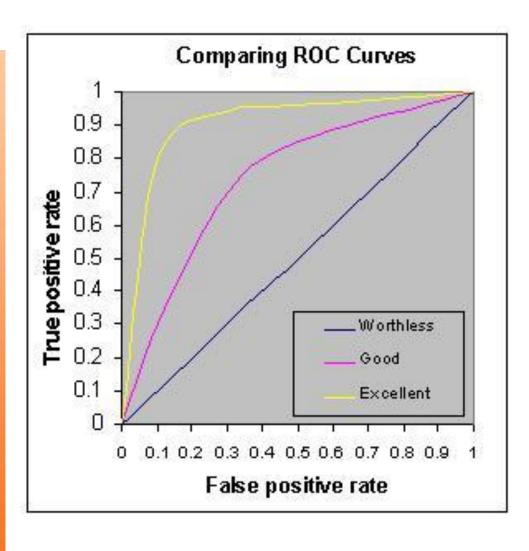




- AUC Measures discrimination, i.e., ability to correctly classify those with and without CHD.
- If you randomly pick <u>one</u> person who HAS CHD and <u>one</u> who DOESN'T and run the model, the one with the higher probability should be from the high risk group.
- AUC is the percentage of randomly drawn such pairs for which the classification is done correctly.







#### Rough rule of thumb:

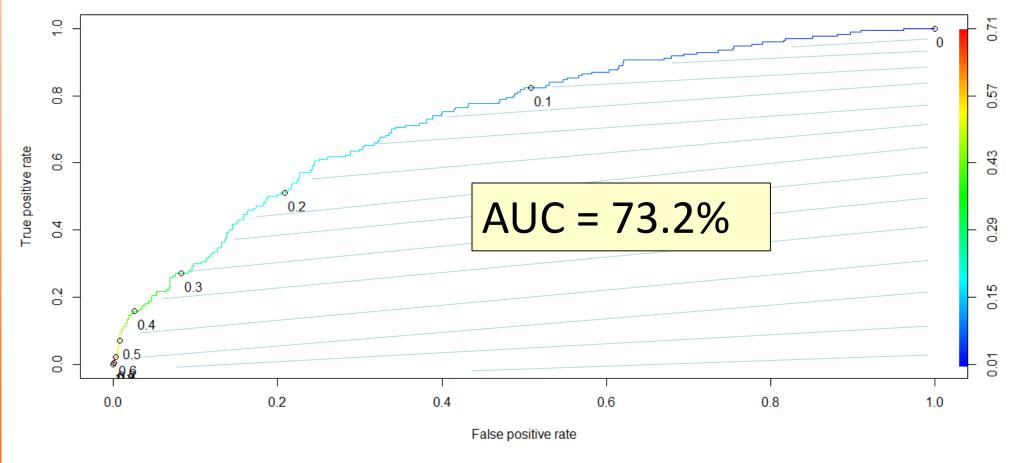
- 0.90 -1.0 = Excellent
- 0.80 0.90 = Good
- 0.70 0.80 = Fair
- 0.60 0.70 = Poor
- 0.50 0.60 = Fail

• <0.50 – You are better off doing a coin toss than working hard to build a model ☺





- The model does a fair job of discrimination between high risk and low risk people.
- Useful for comparing different models.





- In some business problems, it is not good enough to just classify. For
  example, in direct mail or phone marketing campaigns, where it costs
  money to send a mail to each prospect, it is better to be able to rank the
  prospective buyers by their probability to buy. That way, you can order
  them and start calling or mailing them in their decreasing order of
  propensity to buy.
- Lift is a measure of the effectiveness of a predictive model calculated as the ratio between the results obtained with and without the predictive model (random selection).





- A Lift Chart describes how well a model ranks samples in a particular class.
- The greater the area between the lift curve and the baseline (random selection), the better the model.





- A company sends mail catalogs to prospective buyers. It costs the company \$1 to print and mail one catalog.
- From past data, they know the response rate is 5%, i.e., if 100,000 prospective customers are contacted, 5000 buy.
- This means that if there is no model and the company randomly contacts the prospects, they will have the following result.

No. of customers contacted	No. of responses
10000	500
20000	1000
30000	1500
•	
•	
•	
100000	5000



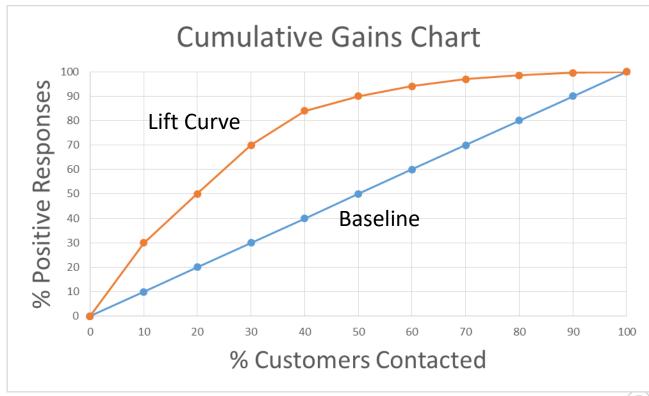
 With a predictive model, where the model assigns a probability to each customer, the customers are ordered and divided into deciles (or any other quantiles). They are then called in decreasing order of probability to buy.

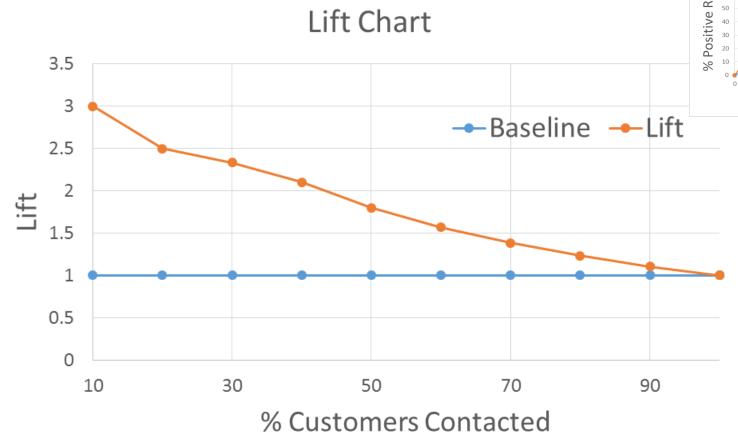
Cost (\$)	Decile contacted	Cumulative responses
10000	10 (top decile)	1500
20000	9	2500
30000	8	3500
40000	7	4200
50000	6	4500
60000	5	4700
70000	4	4850
80000	3	4925
90000	2	4975
100000	1	5000

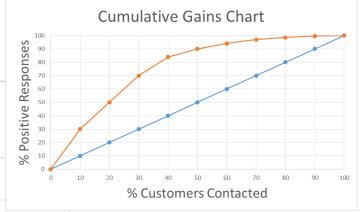


% Called	Called at Random	Called According to Model Score
0	0	0
10	10	30
20	20	50
30	30	70
40	40	84
50	50	90
60	60	94
70	70	97
80	80	98.5
90	90	99.5
100	100	100

Decile contacted	Cumulative responses
10 (top decile)	1500
9	2500
8	3500
7	4200
6	4500
5	4700
4	4850
3	4925
2	4975
1	5000
	10 (top decile) 9 8 7 6 5 4 3







- Max lift of 3 at the top decile.
- Model advantage diminishes as more customers are contacted, especially in lower deciles.
- Useful to compare different models.





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### Classification

# **NAÏVE BAYES ALGORITHM**





### **Classification Problems with Multiple Classes**

- Given an article, predict which section of the newspaper (Current News, International, Arts, Sports, Fashion, etc.) it is supposed to go to
- Given a photo of a car number plate, identify which state it belongs to
- Given an audio clip of a song, identify the genre
- Given an email, predict whether it is spam or not spam (a 2-class problem)





# **Classification Problems**

- All classification problems are essentially equivalent to evaluating conditional probability
- $P(Y_i \mid X)$ , i.e., given certain evidence X, what is the probability that this is from class  $Y_i$
- Logistic Regression solves this problem by modelling the probabilistic relationship between X and Y (sigmoid function, linear in X, etc.)
   directly
- Such models are called <u>Discriminative Models</u>





# **Naïve Bayes Algorithm**

- Naïve Bayes computes P(Y<sub>i</sub> | X) by using Bayes theorem (computes the joint probability - inverse conditional probability P(X | Y<sub>i</sub>) times the prior)
- These type of methods are called <u>Generative Learning</u>
   <u>Models</u>
- A simple classifier that performs surprisingly well on a large class of problems





# **US House of Congress Voting Patterns**

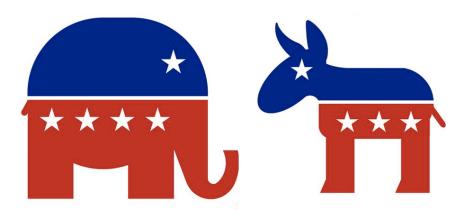
Class	V1	V2	V3	V4	V5	V6	V7	1	Class Name: 2 (democrat, republican)
republican	n	У	n	У	У	У	n	2	handicapped-infants: 2 (y,n)
republican	n	У	n	У	У	У	n	3	
democrat	NA	У	У	NA	У	У	n		J J J
democrat	n	У	У	n	NA	У	n	4	adoption-of-the-budget-resolution: 2 (y,n)
democrat	У	У	У	n	У	У	n	5	physician-fee-freeze: 2 (y,n)
democrat	n	У	У	n	У	У	n	6	el-salvador-aid: 2 (y,n)
democrat	n	У	n	У	У	У	n	7	religious-groups-in-schools: 2 (y,n)
republican		У	n	У	У	У	n		anti-satellite-test-ban: 2 (y,n)
republican	n	У	n	У	У	У	n		W - /
democrat	У	У	У	n	n	n	У	9	aid-to-nicaraguan-contras: 2 (y,n)
republican		У	n	У	У	n	n	10	mx-missile: 2 (y,n)
republican	n	У	n	У	У	У	n	11	immigration: 2 (y,n)
democrat	n	У	У	n	n	n	У	12	,
democrat	У	У	У	n	n	У	У	12	
republican	n	У	n	У	У	У	n	13	education-spending: 2 (y,n)
republican	n	У	n	У	У	У	n	14	superfund-right-to-sue: 2 (y,n)
democrat	У	n	У	n	n	У	n	15	crime: 2 (y,n)
democrat	У	NA	У	n	n	n	У	16	
republican	n	У	n	У	У	У	n	10	duty-free-exports: 2 (y,n)
democrat	У	У	У	n	n	n	У	17	export-administration-act-south-africa: 2 (y,n)

House Votes 1984 Dataset: Voting patterns of Members of Congress.

A data frame with 435 observations on 17 variables. 168 Republicans, 267 Democrats



# Republican or Democrat?



Republican – R – Red Democrat – D - Donkey

**Given** a Congressman's voting pattern (v1 = y, v2 = n), what is the probability that this person is a Democrat?

$$P(D \mid v1 = y, v2 = n) = ?$$



# **Prior Belief - Simplest Solution**

- The house has a majority of Democrats
  - 168 Republicans, 267 Democrats

- Probability of a random person being Democrat is
  - -P(D) = 267/435 = 0.61

 Can we do better by incorporating the evidence of their voting patterns?



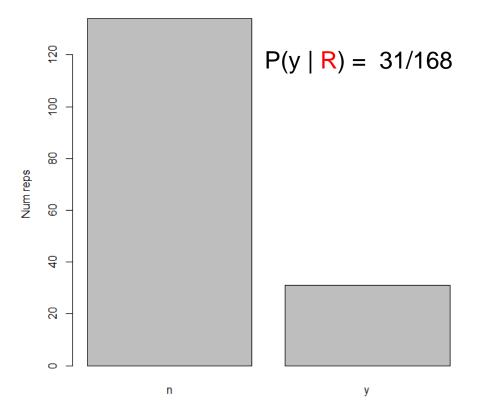


# **Voting Patterns for V1**

Handicapped Infants. The vote failed to pass: 236 to 187

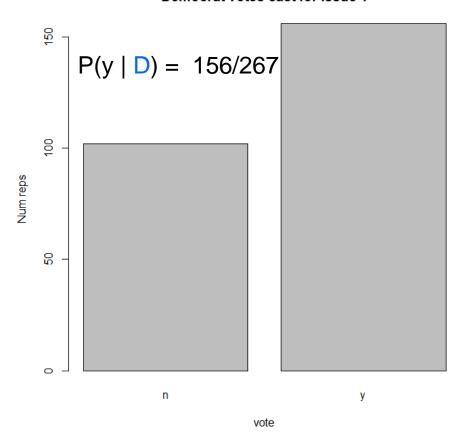
```
> Repub <- HouseVotes84$Class=="republican"
> Democrat <- HouseVotes84$Class=="democrat"
> plot(as.factor(HouseVotes84[Repub,2]))
> title(main="Republican votes cast for issue 1", xlab="vote", ylab="Num reps")
> plot(as.factor(HouseVotes84[Democrat,2]))
> title(main="Democrat votes cast for issue 1", x lab="vote", ylab="Num reps")
```

#### Republican votes cast for issue 1



vote

#### Democrat votes cast for issue 1

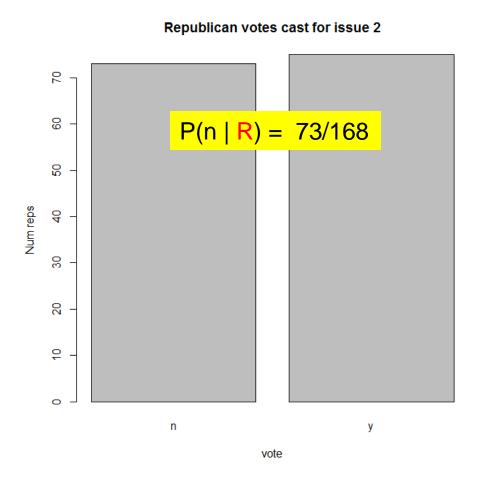


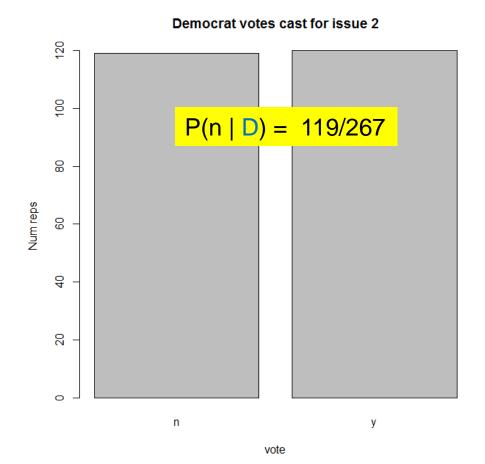


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# **Voting Patterns for V2**

Water-project-cost-sharing. The vote passed: 195 to 192









# **Bayes Theorem**

$$P(A|B) = \frac{P(A) * P(B|A)}{P(B)}$$

$$P(D|v1 = y, v2 = n) = ?$$

$$P(D|v1 = y, v2 = n) = \frac{P(D) * P(v1 = y, v2 = n|D)}{P(v1 = y, v2 = n)}$$





# **Naïve Bayes**

Naïve Assumption: Conditional probability of each feature given the class, is independent of all other features

$$P(v1 = y, v2=n | D) = P(v1 = y | D) * P(v2 = n | D)$$

$$P(D|v1 = y, v2=n) = \frac{P(D) * P(v1 = y|D) * P(v2 = n|D)}{P(v1 = y, v2=n)}$$





# **Naïve Bayes**

We are trying to decide, given the voting pattern, if that person is a Democrat or a Republican.

$$P(D|v1 = y, v2=n) = \frac{P(D) * P(v1 = y|D) * P(v2 = n|D)}{P(v1 = y, v2=n)}$$

$$P(R|v1 = y, v2=n) = \frac{P(R) * P(v1 = y|R) * P(v2 = n|R)}{P(v1 = y, v2=n)}$$

Whichever probability is higher, we would classify the person into that party.

Note that the denominator is the same for both. So we need to focus only on numerator.





# **Naïve Bayes**

$$P(D|V1 = y, V2=n) \propto P(D) * P(V1 = y|D) * P(V2 = n|D)$$

P(D) = 267/435 (267 Democrats among 435 Congressmen)

$$P(D|V1 = y, V2=n) \propto \frac{267}{435} * \frac{156}{267} * \frac{119}{267} = 0.15$$



$$P(R|v1 = y, v2=n) \propto \frac{168}{435} * \frac{31}{168} * \frac{73}{168} = 0.03$$

Since the conditional probability for being Democrat is higher, he is likely to be Democrat.





# Naïve Bayes: Voting patterns



```
library(e1071)
```

```
nb_model <- naiveBayes(Class~.,data = trainHouseVotes84)</pre>
Naive Bayes Classifier for Discrete Predictors
Call:
naiveBayes.default(x = X, y = Y, laplace = laplace)
A-priori probabilities:
  democrat republican
 0.6111111 0.3888889
Conditional probabilities:
            0.4066986 0.5933014
  democrat
  republican 0.8195489 0.1804511
           ٧2
                    n
            0.5119617 0.4880383
  democrat
  republican 0.4586466 0.5413534
```







# **Naïve Bayes Assumption**

 The key assumption of independence of features, is almost never true

Still Naïve Bayes does surprisingly well in a lot of situations

 It works best when all the predictor variables are categorical variables

 Very frequently used in text mining, character image analysis problems





# Evaluating Model Accuracy BIAS-VARIANCE TRADEOFF





# The Ultimate Test of Model Accuracy

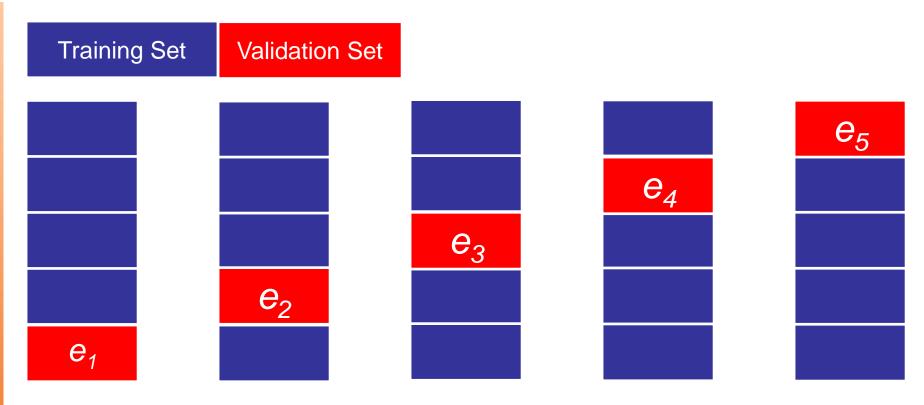
- Holdout set: Split data into train, validation and test sets (in 70:20:10 or 60:20:20, etc. ratios), and ensure model performance is similar.
  - Training Set: For fitting a model
  - Validation Set: For selecting a model based on estimated prediction errors
  - Test Set: For assessing selected model's performance on "new" data





### k-fold Cross-Validation

Common values of *k* are 5 to 10.







#### k-fold Cross-Validation

#### A good model will have

- a small mean of the errors (low bias, i.e., the model accurately captures the behaviour of the data), and
- a small standard deviation of the errors (low variance, i.e., error does not vary much based on the choice of the dataset)





# **Appropriate Error Measures for Evaluating Model Accuracy**

- Use accurate measures of prediction error, experiment with different models and use the model with minimum error.
- Some measures for comparing models within the same technique (e.g., Linear Regression):
  - R<sup>2</sup>
  - AIC





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# **Appropriate Error Measures for Evaluating Model Accuracy**

Some measures for comparing models across techniques:

- MAE (Mean Absolute Error): Mean of the absolute value of the difference between the predicted and actual values.
- MAPE (Mean Absolute Percentage Error): Same as above but converted into percentages to allow for comparison across different scales (e.g., comparing accuracies of forecasts on BSE vs NSE).
- RMSE (Root Mean Square Error): Accounts for infrequent large errors, whose impact may be understated by the mean-based error measures.



 Total error is composed of Bias, Variance and a Random irreducible error. Bias and Variance can be managed.

 If the model performance on training and testing data sets is inconsistent, it indicates a problem either with Bias or Variance.





- Bias arises when you make assumptions preventing you from finding relevant relationships between inputs (independent variables) and outputs (dependent variable). This causes the model to *underfit* the data. For example, assuming linearity when there is non-linearity in the data.
- Variance arises due to the model being overly sensitive to small fluctuations in the training data. Such a model overfits the data, including the random noise rather than just the actual behaviour.





An ideal model will both capture the patterns in the <u>training</u> data and generalize well enough to the <u>unseen (testing)</u> data.

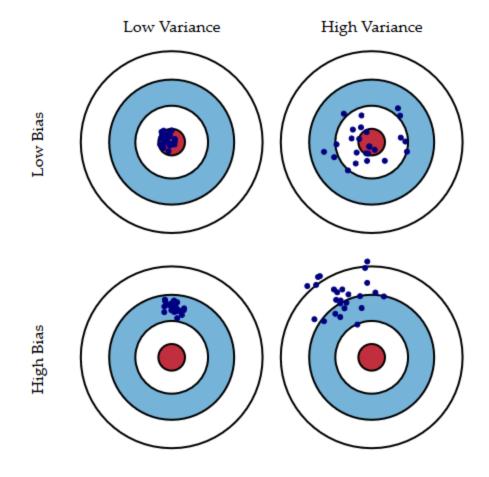
 Unfortunately, it is generally impossible to do both and hence the tradeoff.

 All supervised models (classification, regression, etc.) are affected by this.





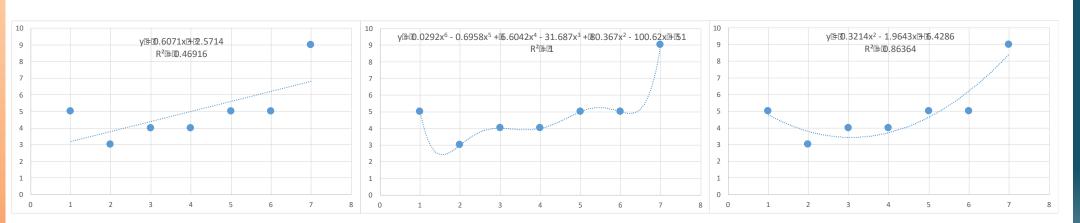
- Bulls-eye is a model that correctly predicts the real values.
- Each hit is a model based on chance variability in training datasets.







# Bias-Variance Tradeoff and Underfitting vs Overfitting Excel

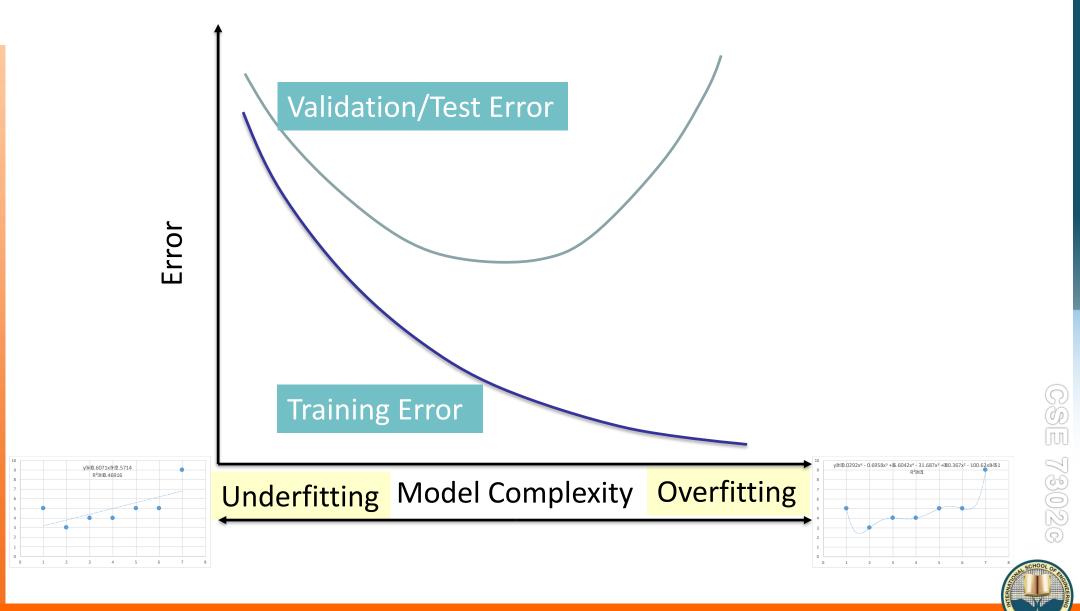


Too Simple a Model Underfit Too Complex a Model
Overfit

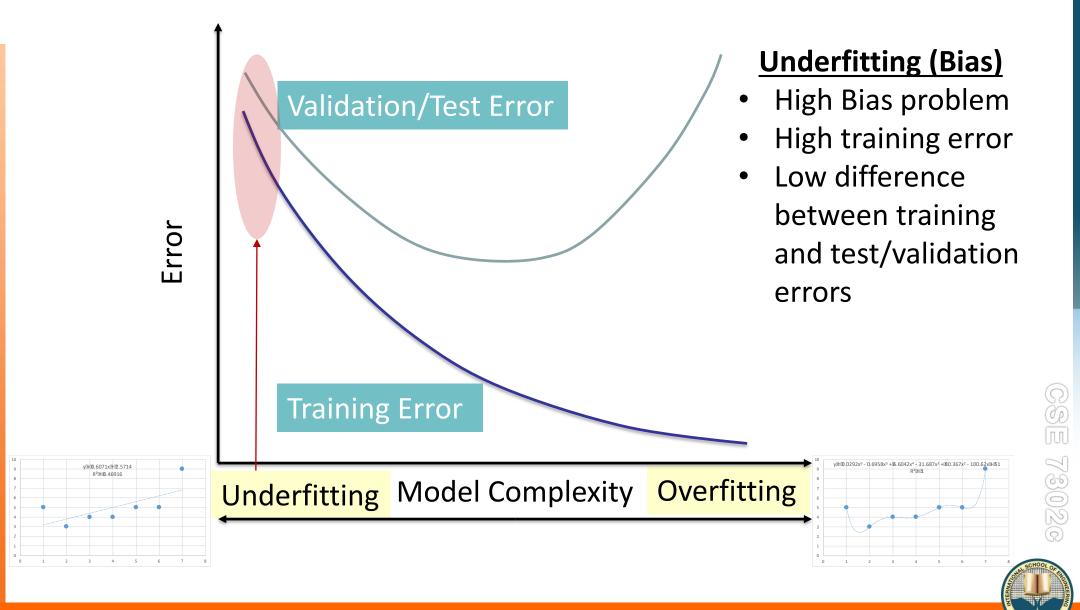
Right Model Reasonable fit



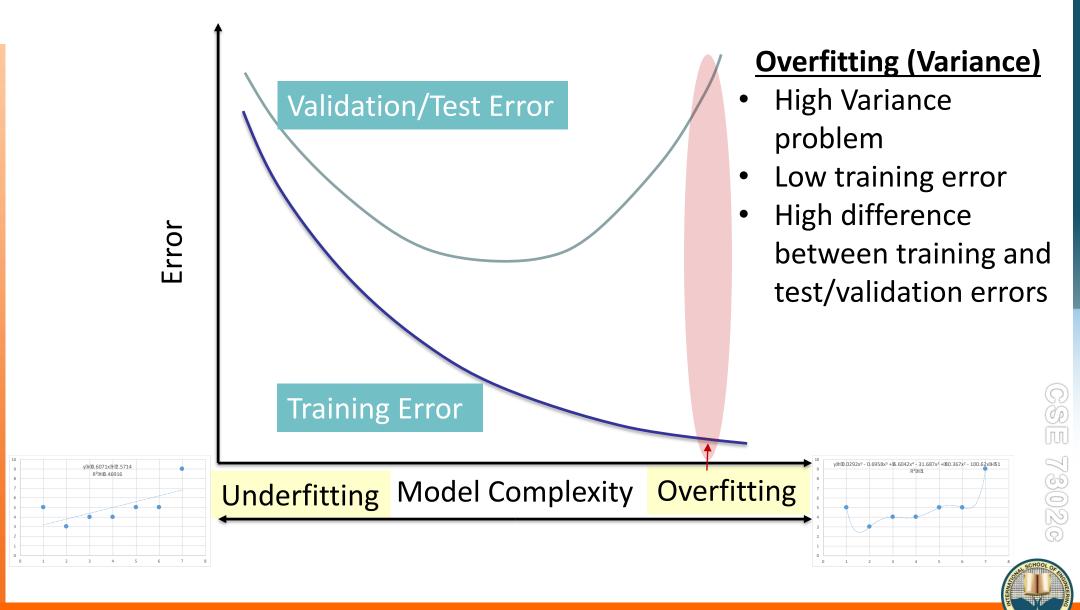
#### **Bias-Variance Tradeoff and Underfitting vs Overfitting**



#### **Diagnosing Bias and Variance**



#### **Diagnosing Bias and Variance**



#### Ways of detecting and minimizing Bias and Variance

- Outliers and Influential Observations can cause statistical bias. Can be identified using various methods like Box plots, points outside  $\pm 2~or~\pm 3$  standard deviations/errors, residual plots, etc.
- Bias cannot be corrected by increasing training sample size.
- Adding features (independent variables or predictors) tends to decrease bias.
- Variance or standard error can be minimized by increasing training sample size.
- Dimensionality reduction and feature selection methods decrease variance.





#### Ways of detecting and minimizing Bias and Variance

Parameters can be tuned in supervised models to control bias and variance:

- Regularization decreases variance at the cost of increasing bias. It can be applied to a variety of techniques (not just linear models).
- In Artificial Neural Networks, bias decreases at the cost of increasing variance with addition of hidden units.
- In kNN, increasing k lowers variance at the cost of increasing bias.
- In Decision Trees, increasing the length of the tree increases variance. Pruning is used to control variance.

Ref: https://en.wikipedia.org/wiki/Bias%E2%80%93variance\_tradeoff

Last accessed: July 08, 2017



#### Ways of detecting and minimizing Bias and Variance

Ensemble models help resolve the tradeoff (taught later in the program).

- Boosting methods combine many "weak" (high bias) models in an ensemble that lowers bias compared to individual models.
- Bagging (bootstrap aggregating) techniques combine "strong" models to minimize variance.

Ref: https://en.wikipedia.org/wiki/Bias%E2%80%93variance\_tradeoff



Last accessed: July 08, 2017







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