Inspire…Educate…Transform.

Statistics and Probability in Decision Modeling

Logistic Regression, ROC and AUC, Gains and Lift Charts, Bias-Variance Tradeoff, Regularization

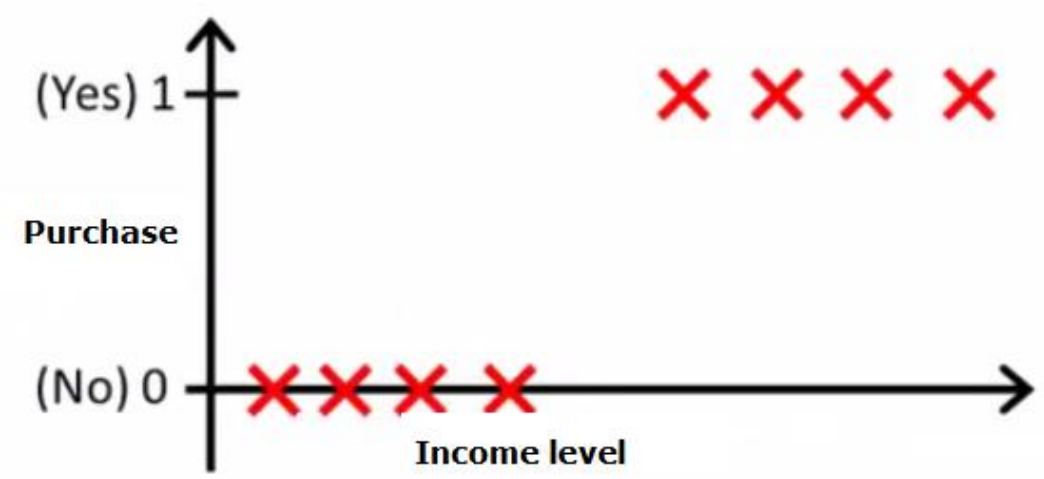
Dr. Venkatesh Sunkad

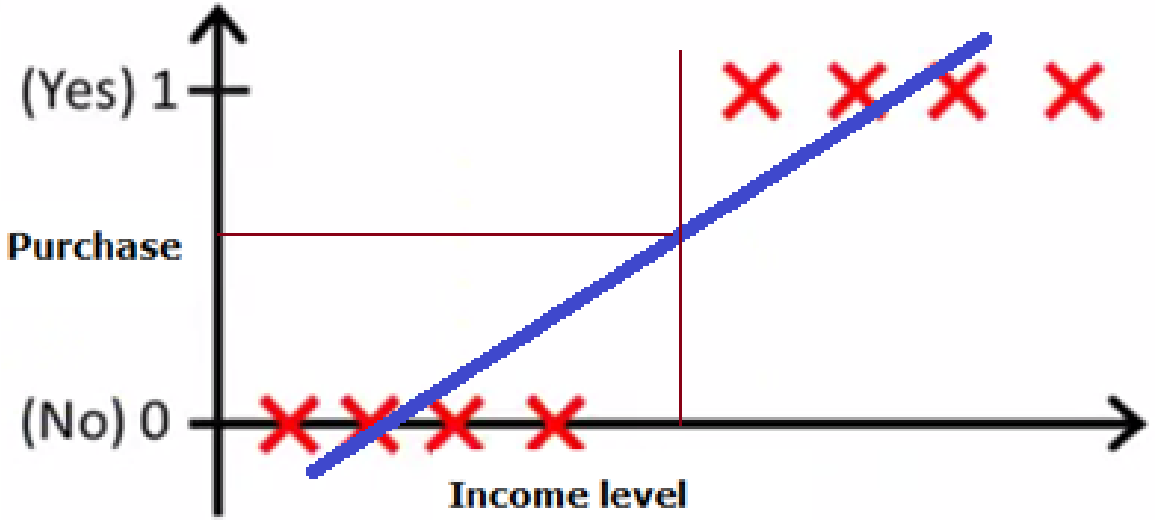
Jan 6 2018

Regularization slides courtesy Dr. Anand Jayaraman

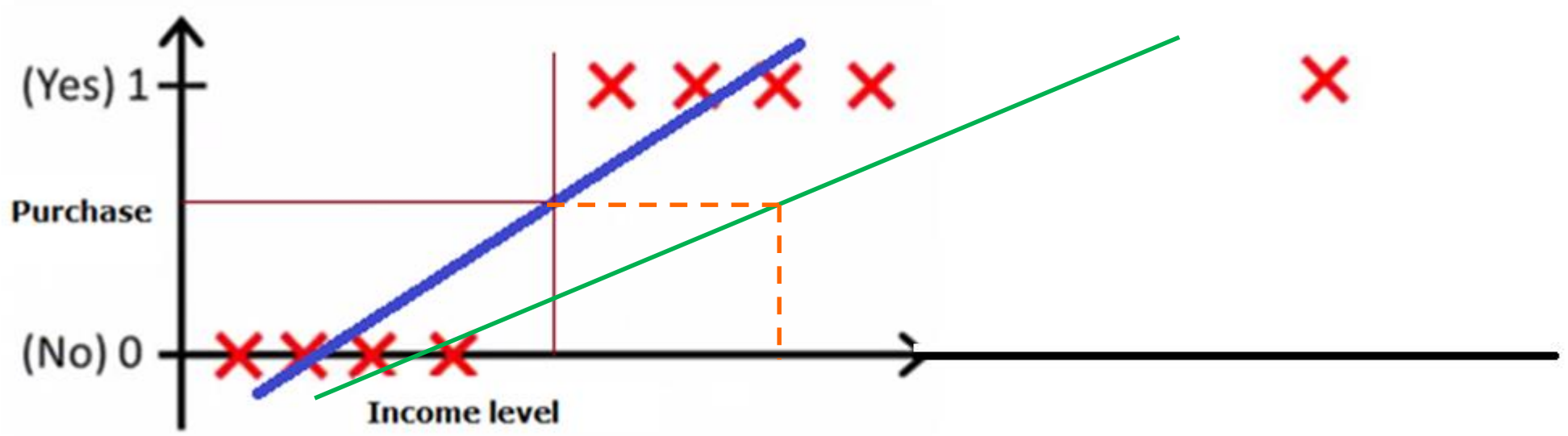
LOGISTIC REGRESSION

Classification Tasks: Regression

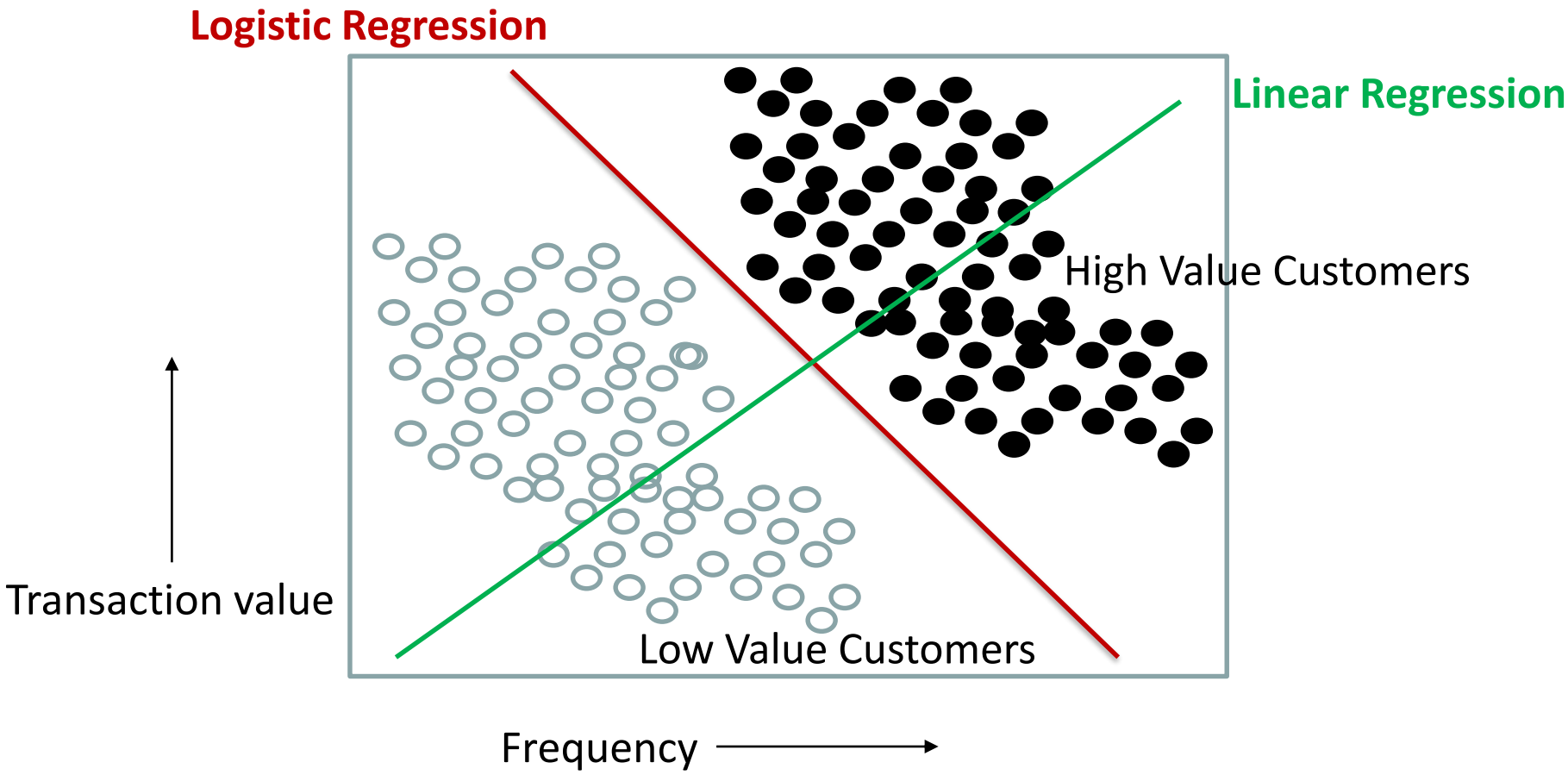




It could fail



Logistic Regression



In addition, linear regression outputs values in the entire range of [-∞, ∞], whereas the actual values in this case are bound by 0 and 1.

That is, $\mathrm{E}(\mathrm{Y}|\mathrm{X} = \mathrm{x}) = \hat{y} = \beta_0 + \beta_1 x_1 + \cdots$ is not useful for such classification tasks. We need a function that can output values between 0 and 1.

A sigmoid or a logistic function allows that, and hence the name Logistic Regression.

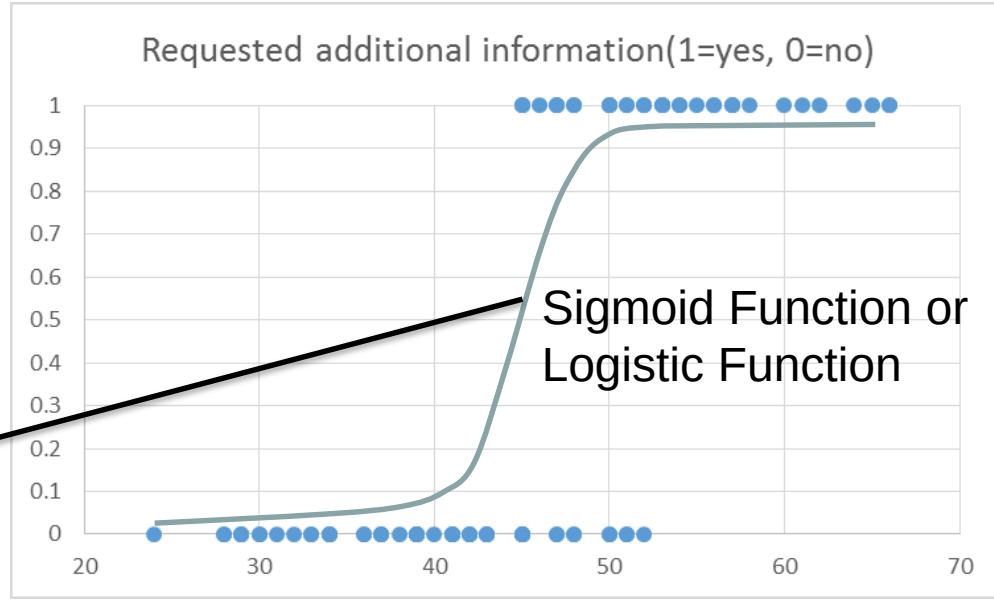
Logistic Regression

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?

Logistic model

$$E(Y|X=x) = f(x) = P(Y=1|X=x) = \frac{1}{1+e^{-\mu}} = \frac{e^{\mu}}{1+e^{\mu}}$$



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

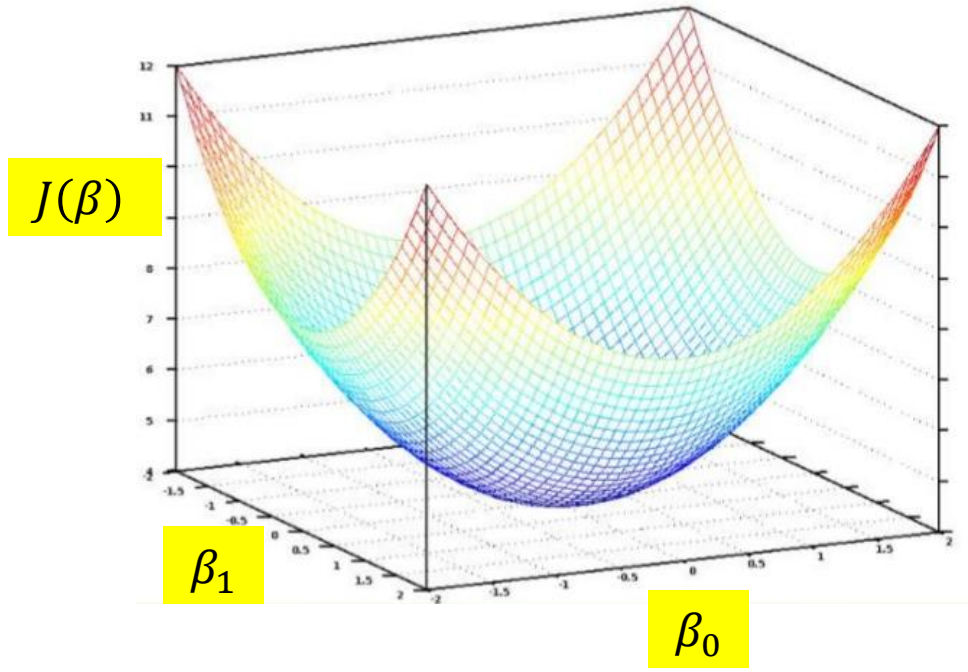
Note: For simplicity, we will use "p" to represent the above conditional probabilities going forward. Please keep in mind that "p" is a nonlinear function of βs.

This is a logistic model. We need to find the optimum β parameters.

Cost Function or Loss Function

In OLS Regression, parameters β were obtained so as to minimize the Cost Function or the Loss Function (squared errors in this case),

$$J(\beta) = \frac{\sum_{i=1,j=1}^{i=n,j=m}\left((\beta_0+\beta_j x_{ij})-y_i\right)^2}{2n}$$, where *n* is the # of observations and *m* are the number of independent variables.



$J(\beta)$ can be minimized using an Analytical/Calculus based approach, which gives the best linear unbiased estimators (βs) when the OLS assumptions are met.

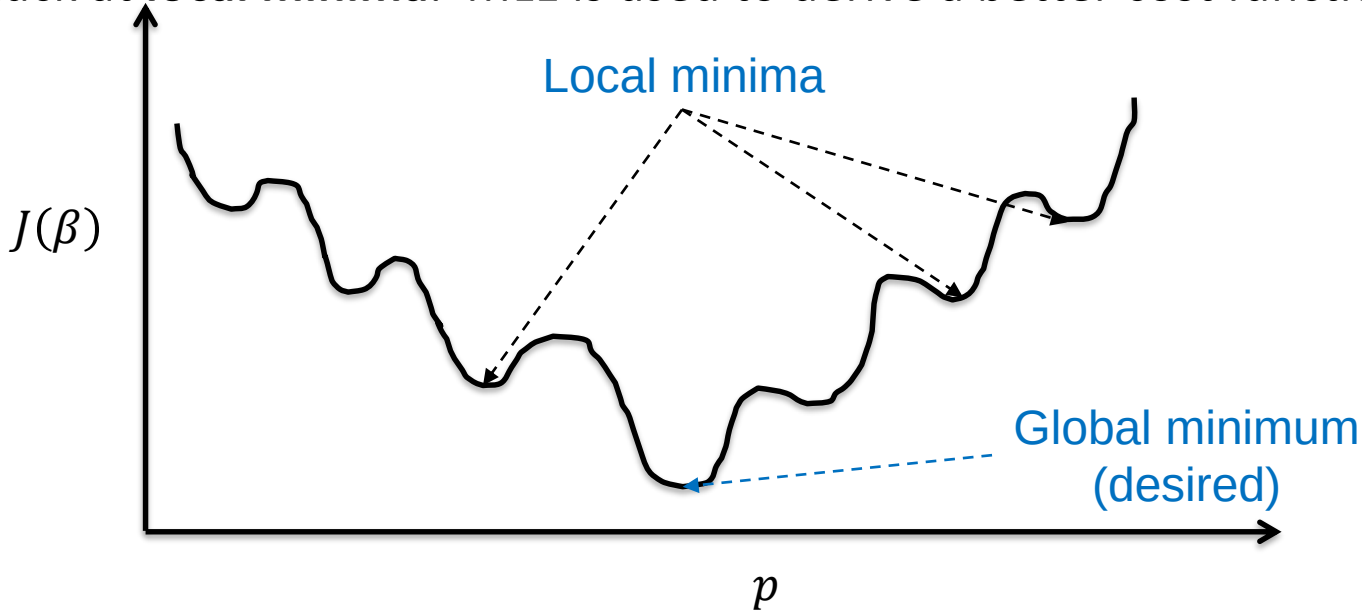
Image source: https://www.slideshare.net/ocampesato/d3-typescript-and-deep-learning
Last accessed: May 18, 2018

Maximum Likelihood Estimation (MLE) Principle to Derive Cost Function in Logistic Regression

A squared errors based cost function in Logistic Regression is highly non-linear leading to various minima because we are using a **non-linear sigmoid function** and then squaring it.

$$J(\beta) = \frac{\sum(p_i - y_i)^2}{2n}$$

The algorithm may get stuck at **local minima**. MLE is used to derive a better cost function.



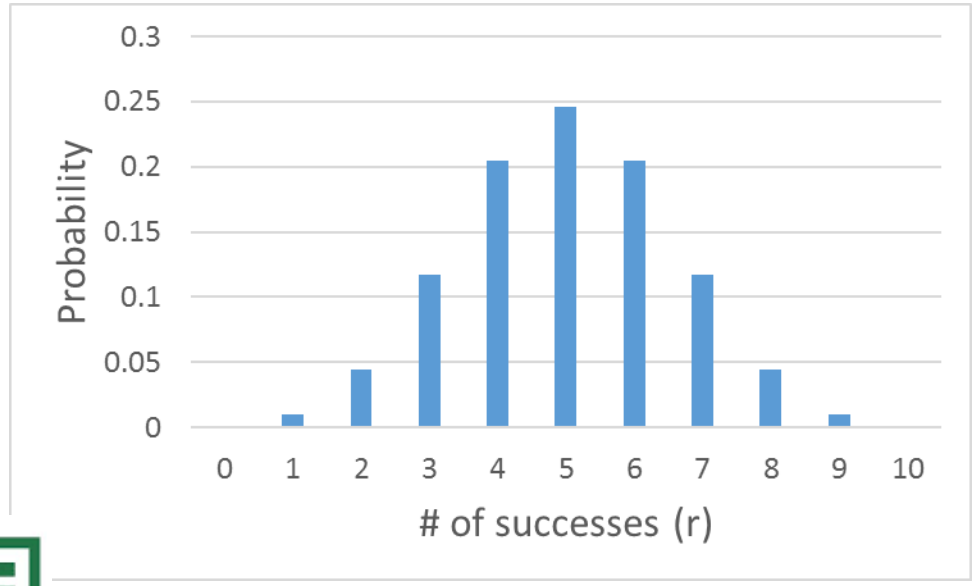
Reference: Andrew Ng's Machine Learning course on Coursera

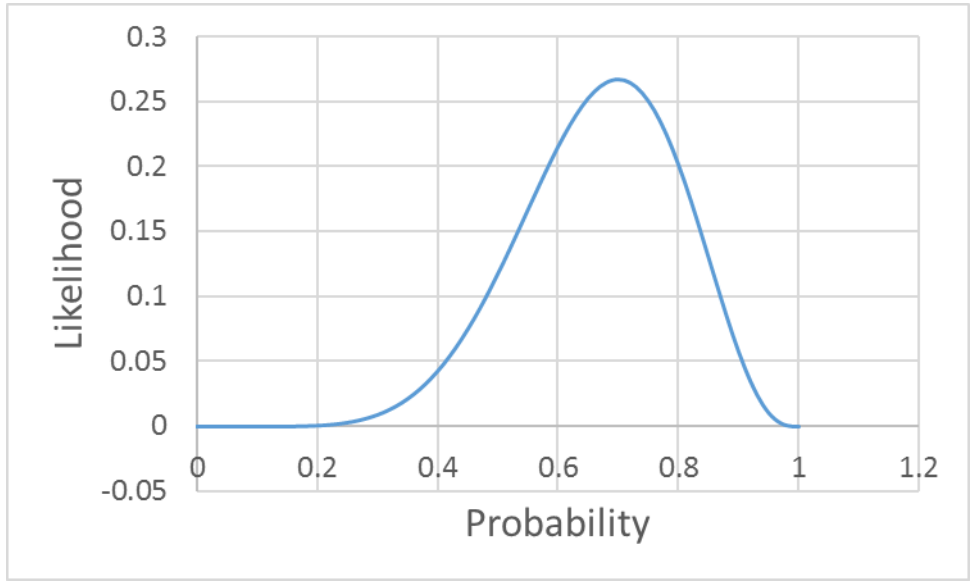
Maximum Likelihood Estimation (MLE)

INTUITION

Probability vs Likelihood – Excel ["Probability –likehood"]

- Likelihood is also known as reverse probability.
- In Probability, we **predict data** based on **known parameters**.
  (Recall B(n,p), Geo(p), Po(λ), N(μ,σ^2), etc.)
- In Likelihood, we **predict parameters** based on **known data**.



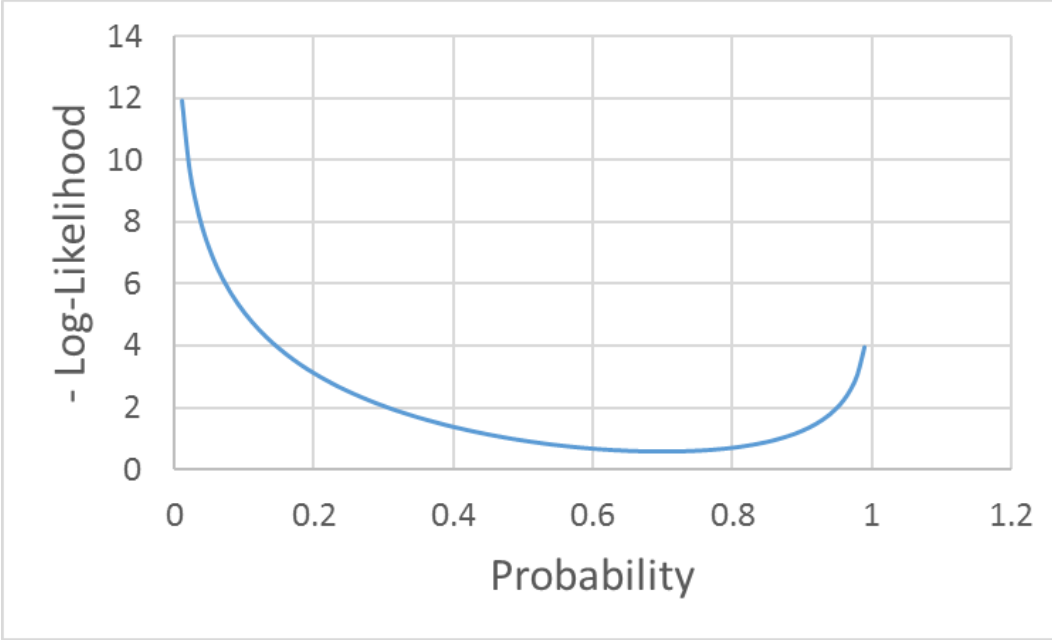


MLE

- Goal is to find parameters that **maximize the likelihood** of our observed data, which is the same as **minimizing errors**.

- We use calculus where functions are simple (minimize sum of squared errors in linear regression, and so on) or numerical techniques like Gradient Descent, Newton's Method, Fisher's Scoring, etc. (minimize deviance in logistic regression, Neural Nets, etc.), which work for both simple and complex functions, but become necessary for complex functions.

- So, Maximum Likelihood => Minimum of Negative Likelihood. That is, negative likelihood, or more specifically, **negative log-likelihood** is a measure of the errors of the model (what the model is unable to explain).



MLE to Derive Logistic Regression Objective and Cost Functions

L: Likelihood
P: Probability
LL: Log-likelihood

We have understood that

$L(Parameters|Observations) = P(Observations|Parameters)$

$\therefore log(L) = log(p)$

Remember, $P(Y=1|X=x) = p$ and $P(Y=0|X=x) = 1-p$

We can write $log(p_{class1}) = 1*log(p) = y_i*log(p)$ because $y_i = 1$ for class1.

Similarly, $log(p_{class2}) = 1*log(1-p) = (1-y_i)*log(1-p)$ because $y_i = 0$ for class2.

As either $y_i=0$ or $(1-y_i)=0$, we can combine the two to write

$log(p) = log(L) = \mathbf{LL = y_i*log(p) + (1-y_i)*log(1-p)}$

This **LL** is the **Objective Function** we want to maximize. This is the same as minimizing the **–LL**, which becomes our **Cost Function**.

Cost Function

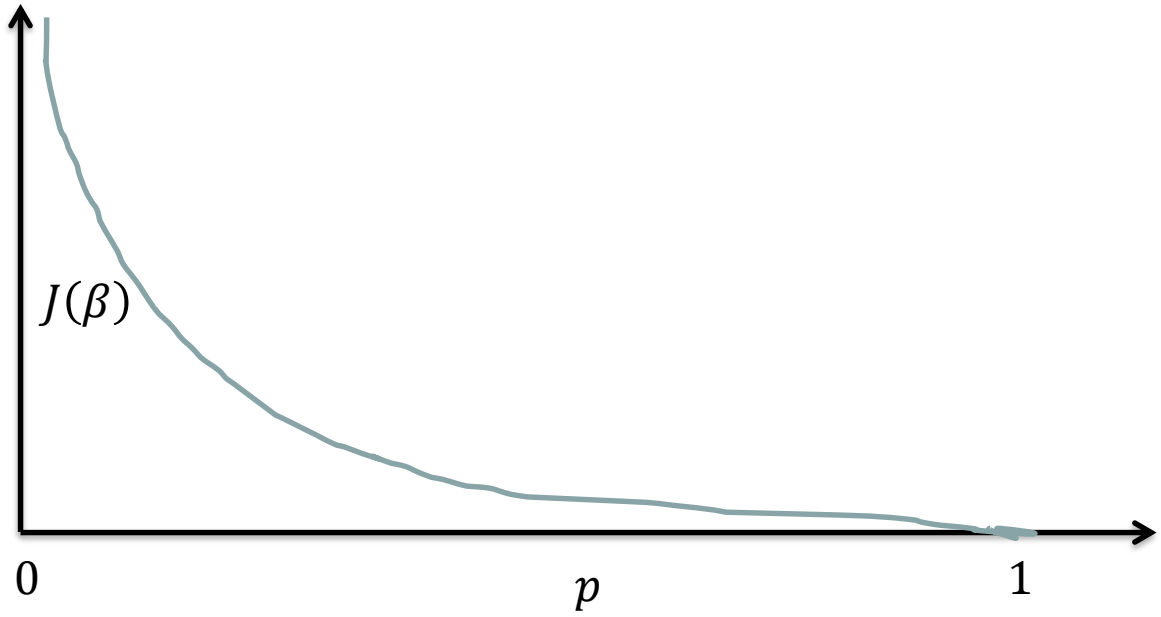
The cost function that provides a nice convex curve with a global minimum is given by:

$$J(\beta) = -\frac{1}{n}\left[\sum_{i=1}^{n} y_i \log(p) + (1 - y_i)\log(1 - p)\right]$$

Note: Don't forget p is the sigmoid function given by $P(Y = 1|X = x) = \frac{1}{1+e^{-\mu}} = \frac{e^{\mu}}{1+e^{\mu}}$, *with* μ *being a linear function of* β*s.*

What is the cost or penalty on the algorithm if $y_i = 1$, and the algorithm predicts with $p = 1$?

What is the cost or penalty on the algorithm if $y_i = 1$, and the algorithm predicts with $p = 0$?



Reference: Andrew Ng's Machine Learning course on Coursera

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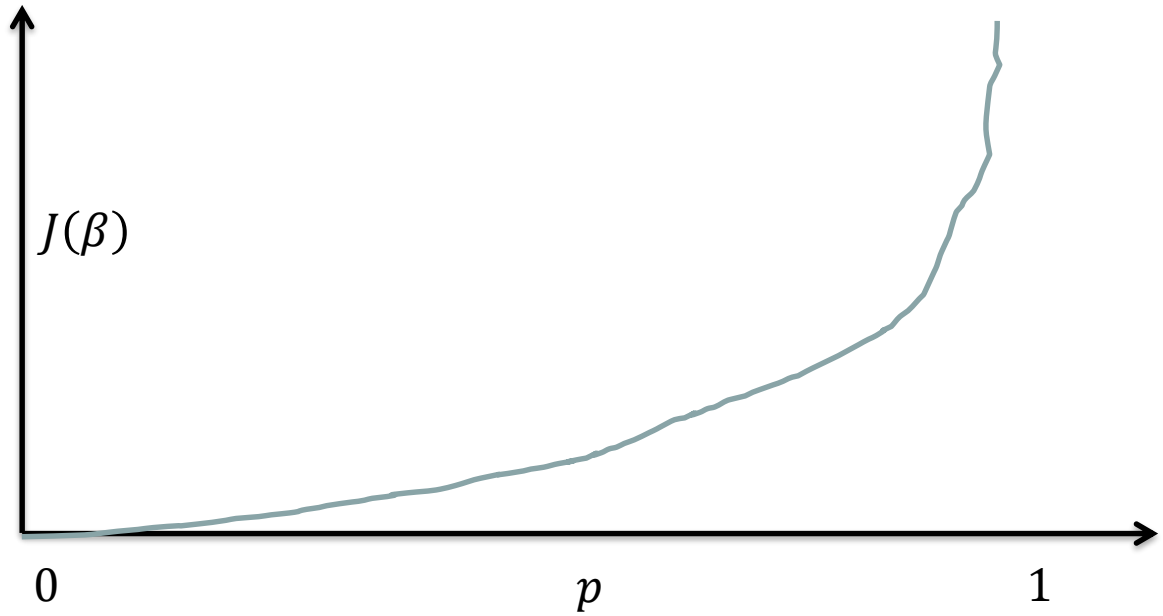
What is the cost or penalty on the algorithm if $y_i = 0$, and the algorithm predicts with $p = 1$?

What is the cost or penalty on the algorithm if $y_i = 0$, and the algorithm predicts with $p = 0$?



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Cost Function

The cost function that provides a nice convex curve with a global minimum is given by:

$$J(\beta) = -\frac{1}{n}\left[\sum_{i=1}^{n} y_i \log(p) + (1 - y_i)\log(1 - p)\right]$$

There is no analytical solution to this, though. *Note p is a sigmoid function.* Algorithms like **Gradient Descent** are used instead.

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

Reference: Andrew Ng's Machine Learning course on Coursera

Maxima and Minima – Gradient Descent

Maxima and Minima – Calculus Approach (Refresher)

$$y = x^3 - 2x^2 + x + 3$$

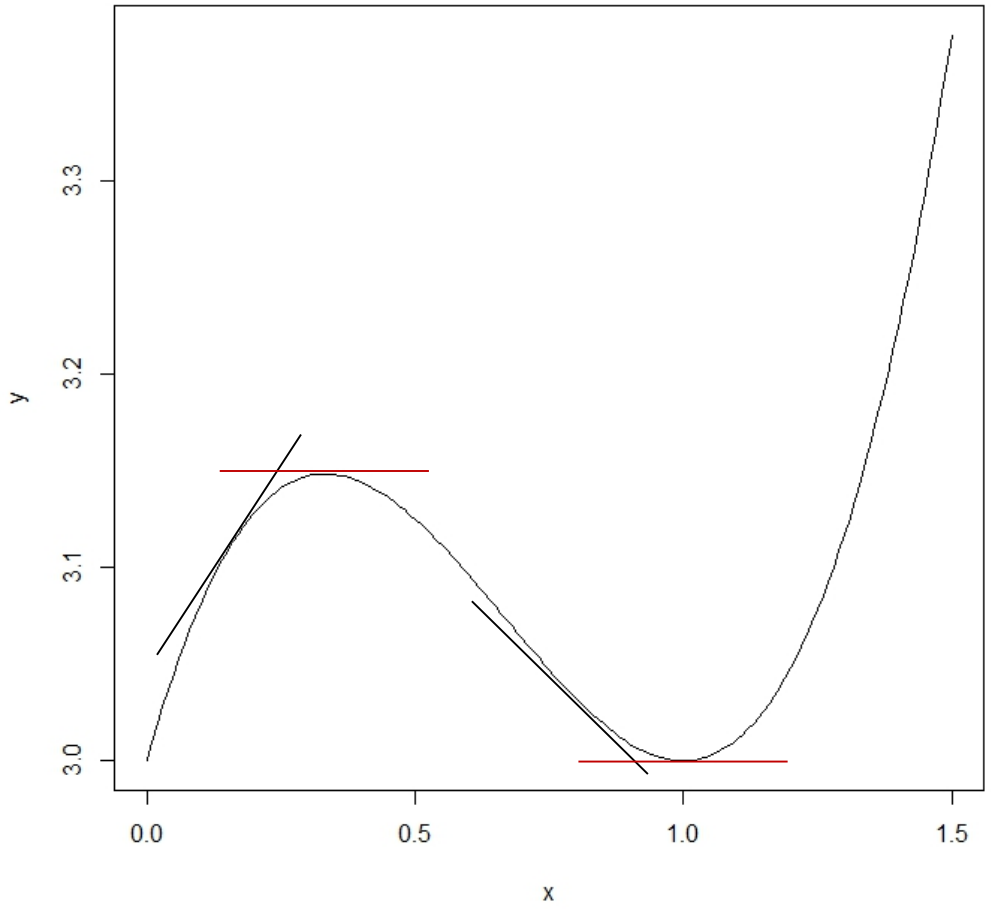
$$\frac{dy}{dx} = 3.x^2 - 4.x + 1 = 0$$

$$\frac{dy}{dx} = 0 \Rightarrow x = \frac{1}{3} \; or \; 1$$

$$\frac{d}{dx}\left(\frac{dy}{dx}\right) = \frac{d^2y}{dx^2} = 6.x - 4$$

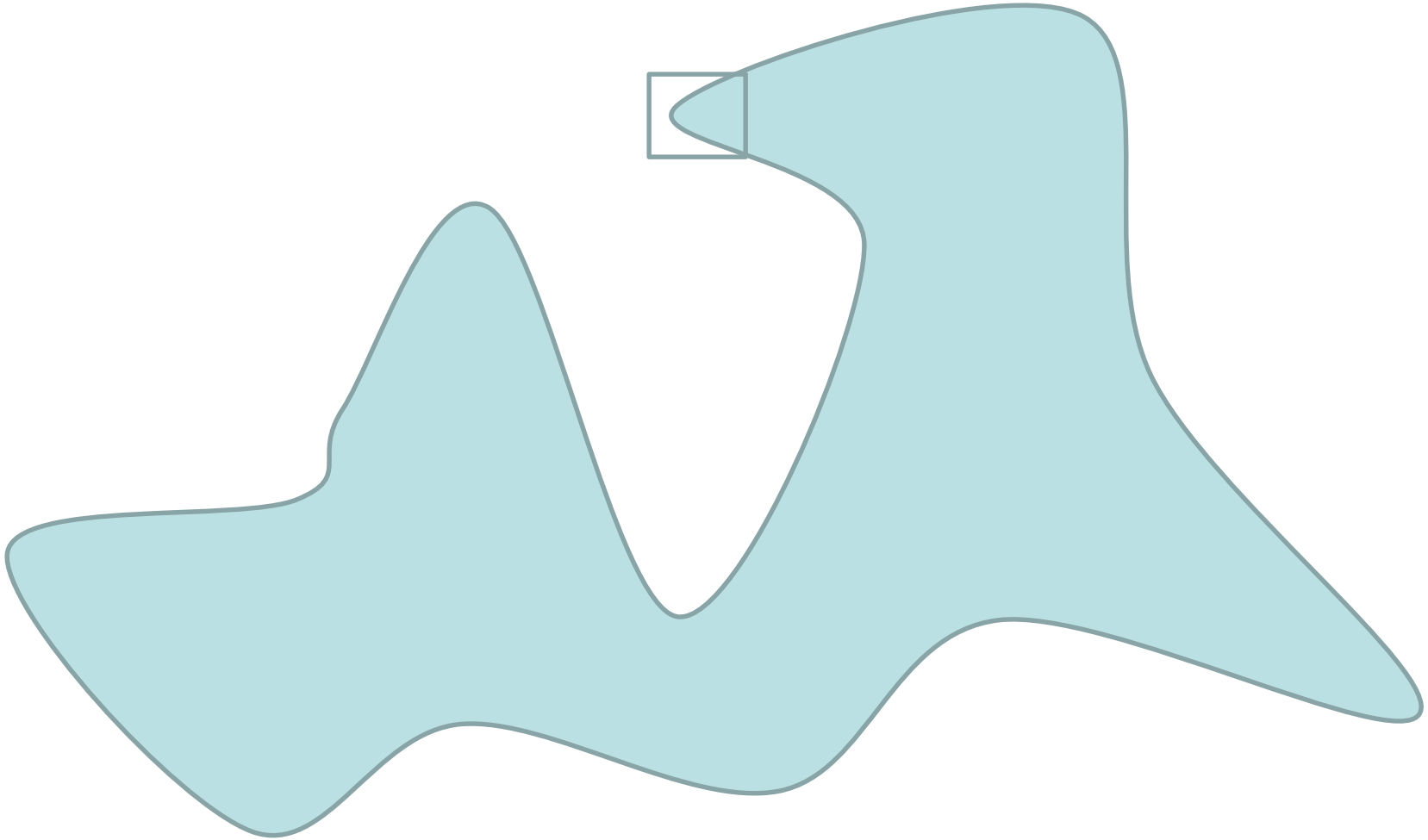
$$for \; x = 1; \frac{d^2y}{dx^2} = 2. \; \text{So}, 1 \; is \; minima$$

$$for \; x = \frac{1}{3}; \frac{d^2y}{dx^2} = -2. \; \text{So}, \frac{1}{3} \; is \; maxima$$



CSE 73026

Finding Maxima and Minima For Extremely Complex Functions – Iterative Numerical Approach

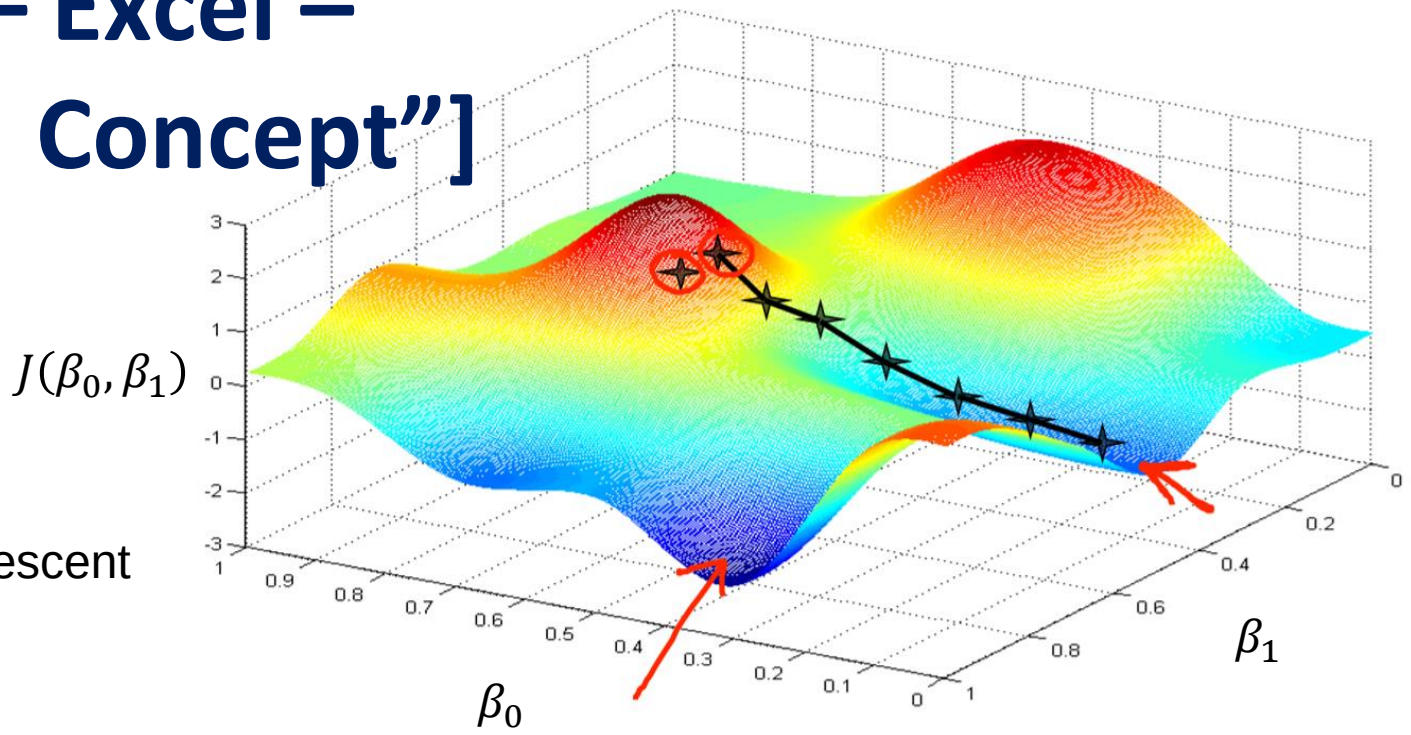


Gradient Descent – Excel – ["Gradient Decent Concept"]

$$\beta_0^{(t+1)} = \beta_0 - \alpha \frac{\partial J(\beta_0, \beta_1)}{\partial \beta_0}$$

Learning Rate

Slope of steepest descent

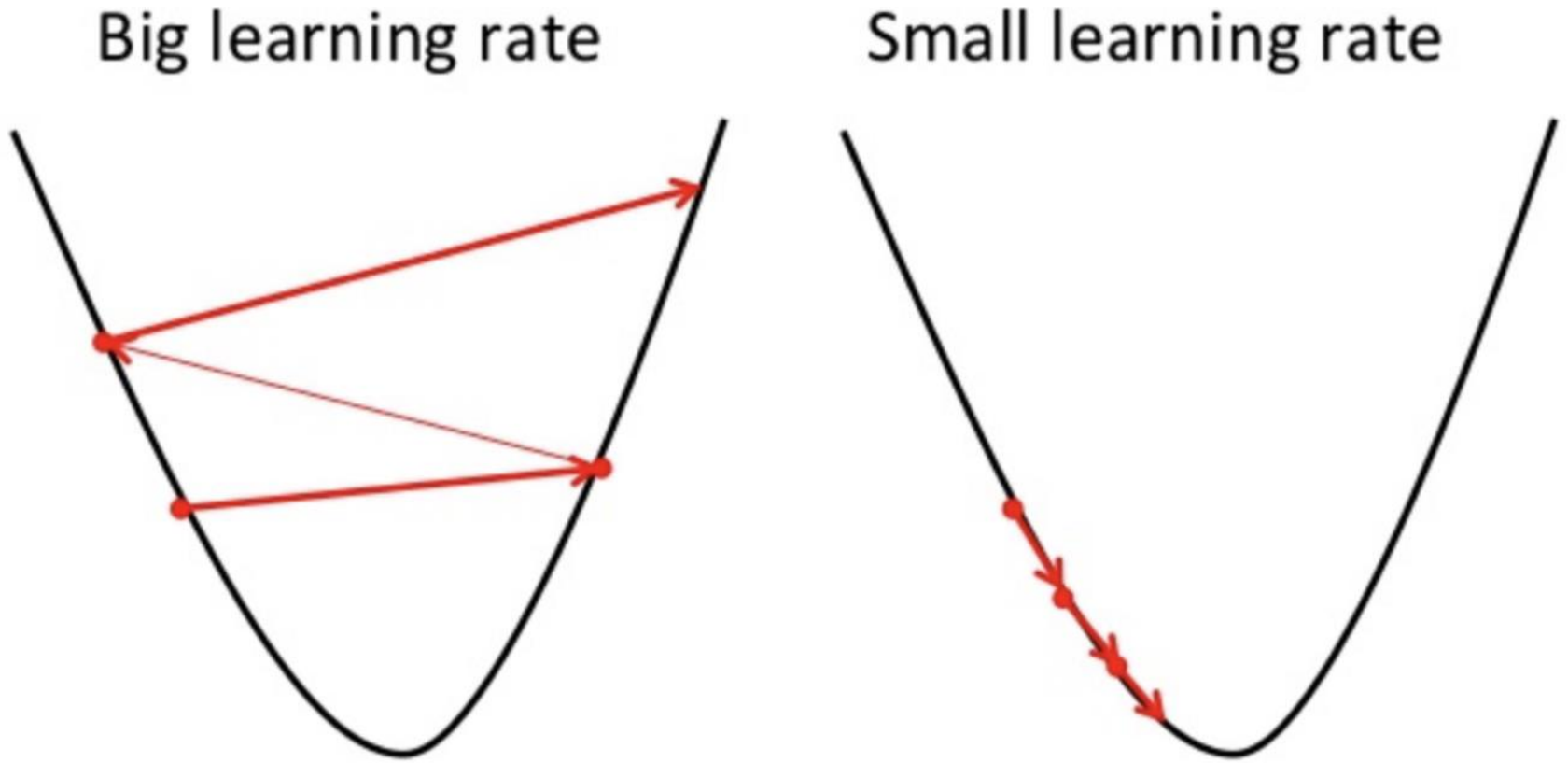


Source: Andrew Ng's Machine Learning course on Coursera

$$\beta_1^{(t+1)} = \beta_1 - \alpha \frac{\partial J(\beta_0, \beta_1)}{\partial \beta_1}$$

Learning Rate

BREAK



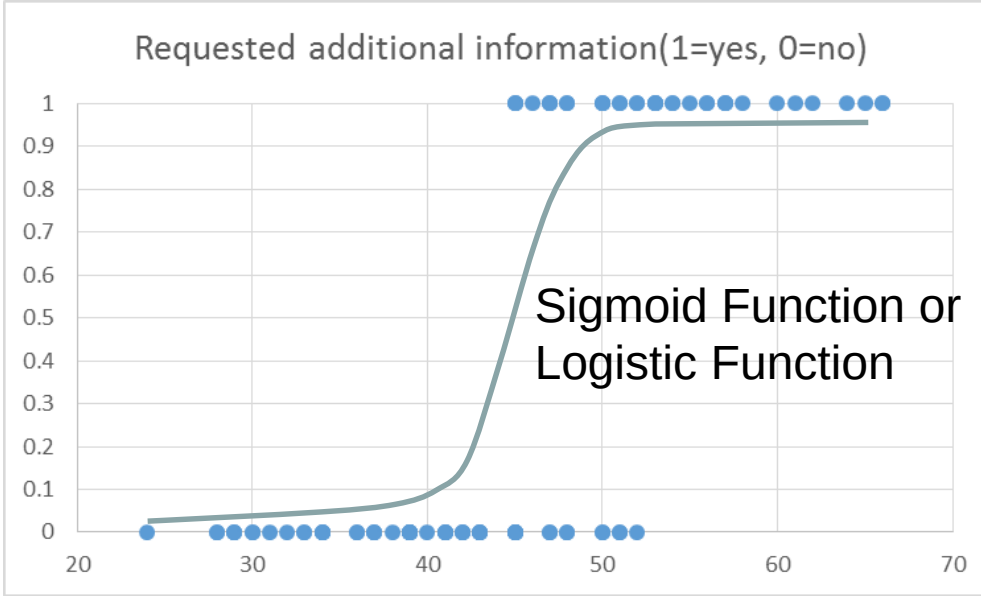
Source: https://towardsdatascience.com/gradient-descent-in-a-nutshell-eaf8c18212f0

Logistic model

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

Logistic model can be transformed into Odds:

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



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

Attention Check – Probability and Odds

If the probability of winning is 6/12, what are the odds of winning?	1:1 (Note, the probability of losing also is 6/12)
If the odds of winning are 13:2, what is the probability of winning?	13/15
If the odds of winning are 3:8, what is the probability of losing?	8/11
If the probability of losing is 6/8, what are the odds of winning?	2:6 or 1:3

$$\text{Odds of winning} = \frac{Probability\ of\ Winning\ (Success)}{Probability\ of\ Losing\ (Failure)}$$

Logistic model

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

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

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

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

Logistic model

The log of the odds is called logit, and the transformed model is linear in βs.

Solving the Logistic regression problem essentially reduces to finding the set of βs that minimizes error.

and Interpreting the output

```
Call:
glm(formula = Response ~ Age, family = "binomial", data = flierresponse)

Deviance Residuals:
     Min        1Q    Median        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 ***
Age           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
```

What is the logit equation?

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

CSE 7302c

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

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

[Remember $S = Odds = \frac{p}{1-p}$]

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

The output of the logistic regression is a probability value. You need to fix a threshold value before a class is assigned.

Computing using R

What is the probability that a 50 year-old will return the form?

```
> flierresponseglm <- glm(Response~Age, data = flierresponse, family = "binomial")
> nd <- data.frame(Age=50)  #To predict the probability for Age=50, put that info in a data-frame
> predict(flierresponseglm,newdata=nd)  # This gives the log-Odds
        1
0.8879707
> predict(flierresponseglm,newdata=nd,type="response")  # Compute the probability
        1
0.7084712
```

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.

$$\boldsymbol{D = -2LL} = -2 * \left[\sum_{i=1}^{n} y_i \log(p) + (1 - y_i) \log(1 - p) \right]$$

where LL is the log-likelihood.

```
Call:
glm(formula = Response ~ Age, family = "binomial", data = flierresponse)

Deviance Residuals:
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```

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.

```
Call:
glm(formula = Response ~ Age, family = "binomial", data = flierresponse)

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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 = nln(RSS/n) + 2k***.
- AIC is *similar to Adjusted* R^2 in the sense it penalizes for adding more parameters to the model.

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

- 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

Framingham Heart Study
A Project of the National Heart, Lung, and Blood Institute and Boston University

- 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)				
Age	**29-39**	**40-49**	**50-62**	**Totals**
Men	835	779	722	2,336
Women	1,042	962	869	2,873
Totals	1,877	1,741	1,591	5,209

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/

Case Study – Data (framinghamheartstudy.org and MITx)

	male	age	education	currentSmoker	cigsPerDay	BPMeds	prevalentStroke	prevalentHyp	diabetes	totChol	sysBP	diaBP	BMI	heartRate	glucose	TenYearCHD
1	1	39	4	0	0	0	0	0	0	195	106.0	70.0	26.97	80	77	0
2	0	46	2	0	0	0	0	0	0	250	121.0	81.0	28.73	95	76	0
3	1	48	1	1	20	0	0	0	0	245	127.5	80.0	25.34	75	70	0
4	0	61	3	1	30	0	0	1	0	225	150.0	95.0	28.58	65	103	1
5	0	46	3	1	23	0	0	0	0	285	130.0	84.0	23.10	85	85	0
6	0	43	2	0	0	0	0	1	0	228	180.0	110.0	30.30	77	99	0
7	0	63	1	0	0	0	0	0	0	205	138.0	71.0	33.11	60	85	1
8	0	45	2	1	20	0	0	0	0	313	100.0	71.0	21.68	79	78	0
9	1	52	1	0	0	0	0	1	0	260	141.5	89.0	26.36	76	79	0
10	1	43	1	1	30	0	0	1	0	225	162.0	107.0	23.61	93	88	0
11	0	50	1	0	0	0	0	0	0	254	133.0	76.0	22.91	75	76	0
12	0	43	2	0	0	0	0	0	0	247	131.0	88.0	27.64	72	61	0
13	1	46	1	1	15	0	0	1	0	294	142.0	94.0	26.31	98	64	0
14	0	41	3	0	0	1	0	1	0	332	124.0	88.0	31.31	65	84	0
15	0	39	2	1	9	0	0	0	0	226	114.0	64.0	22.35	85	*NA*	0
16	0	38	2	1	20	0	0	1	0	221	140.0	90.0	21.35	95	70	1
17	1	48	3	1	10	0	0	1	0	232	138.0	90.0	22.37	64	72	0
18	0	46	2	1	20	0	0	0	0	291	112.0	78.0	23.38	80	89	1
19	0	38	2	1	5	0	0	0	0	195	122.0	84.5	23.24	75	78	0
20	1	41	2	0	0	0	0	0	0	195	139.0	88.0	26.88	85	65	0
21	0	42	2	1	30	0	0	0	0	190	108.0	70.5	21.59	72	85	0
22	0	43	1	0	0	0	0	0	0	185	123.5	77.5	29.89	70	*NA*	0
23	0	52	1	0	0	0	0	0	0	234	148.0	78.0	34.17	70	113	0
24	0	52	3	1	20	0	0	0	0	215	132.0	82.0	25.11	71	75	0
25	1	44	2	1	30	0	0	1	0	270	137.5	90.0	21.96	75	83	0
26	1	47	4	1	20	0	0	0	0	294	102.0	68.0	24.18	62	66	1

Case Study – Predicting Coronary Heart Disease (CHD)

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)

Case Study – Predicting Coronary Heart Disease (CHD)

- 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

Case Study – Predicting Coronary Heart Disease (CHD)

- 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/m^2)
  - *heartRate*: # of beats per minute
  - *glucose*: Blood glucose level (mg/dL)

Case Study – Predicting Coronary Heart Disease (CHD)

Approach

- Randomly split data into training and test in 70:30 ratio.
- Measure prediction accuracies on training and test data
- Although the split is random, make sure the proportions of the categories are roughly the same in both training and test sets.

```
# Randomly split the data into training and testing sets
set.seed(1000)
split = sample.split(framingham$TenYearCHD, SplitRatio = 0.70)

# Split up the data using subset
train = subset(framingham, split==TRUE)
test = subset(framingham, split==FALSE)

# Check the proportions of CHD in both sets
cat(sum(train$TenYearCHD)/nrow(train),sum(test$TenYearCHD)/nrow(test))
```

```
0.1519542 0.1517296
```

Case Study – Predicting Coronary Heart Disease (CHD)

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       1Q   Median       3Q      Max
-1.9392  -0.5998  -0.4211  -0.2771   2.8632

Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
(Intercept)     -8.360272   0.864696  -9.668  < 2e-16 ***
male             0.524080   0.130836   4.006 6.19e-05 ***
age              0.065429   0.008049   8.129 4.34e-16 ***
education       -0.041105   0.059185  -0.695 0.487366
currentSmoker    0.120498   0.187629   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     0.307077   0.166034   1.849 0.064389 .
diabetes        -0.319937   0.392574  -0.815 0.415087
totChol          0.003799   0.001330   2.856 0.004290 **
sysBP            0.011144   0.004446   2.507 0.012188 *
diaBP           -0.001861   0.007760  -0.240 0.810517
BMI              0.008812   0.015662   0.563 0.573702
heartRate       -0.007273   0.005131  -1.418 0.156296
glucose          0.009227   0.002752   3.353 0.000798 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(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
```

Missing Values

There are several ways of dealing with missing values.

If large percentage of data for a given variable is missing, then we don't use that variable for building the model.

If the percentage of missing values is small (5 to 10%)

- Naïve method: Replace the missing values with either mean, median or mode
- Intelligent method: Impute the missing values from the relationship between the variables

Also see: https://www.r-bloggers.com/imputing-missing-data-with-r-mice-package/

VIF, GVIF, GVIF$^{\left(\frac{1}{2*df}\right)}$

Predicting Coronary Heart Disease Case

```
Call:
glm(formula = TenYearCHD ~ ., family = binomial, data = train)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.9392  -0.5998  -0.4211  -0.2771   2.8632

Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
(Intercept)     -8.360272   0.864696  -9.668  < 2e-16 ***
male             0.524080   0.130836   4.006 6.19e-05 ***
age              0.065429   0.008049   8.129 4.34e-16 ***
education       -0.041105   0.059185  -0.695 0.487366
currentSmoker    0.120498   0.187629   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     0.307077   0.166034   1.849 0.064389 .
diabetes        -0.319937   0.392574  -0.815 0.415087
totChol          0.003799   0.001330   2.856 0.004290 **
sysBP            0.011144   0.004446   2.507 0.012188 *
diaBP           -0.001861   0.007760  -0.240 0.810517
BMI              0.008812   0.015662   0.563 0.573702
heartRate       -0.007273   0.005131  -1.418 0.156296
glucose          0.009227   0.002752   3.353 0.000798 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(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
```

- Education as **numeric** variable

```
> framingham = read.csv("framingham.csv")
> str(framingham)
'data.frame':   4240 obs. of  16 variables:
 $ male           : int  1 0 1 0 0 0 0 0 1 1 ...
 $ age            : int  39 46 48 61 46 43 63 45 52 43 ...
 $ education      : int  4 2 1 3 3 2 1 2 1 1 ...
```

- car package gives the following VIF figures

```
> car::vif(framinghamLog)
     male       age     education
 1.247670  1.278996  1.057810
```

CSE 7302c

VIF, GVIF, GVIF$^{\left(\frac{1}{2*df}\right)}$

Predicting Coronary Heart Disease Case

```
Call:
glm(formula = TenYearCHD ~ ., family = binomial, data = train)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.9315  -0.5948  -0.4196  -0.2733   2.8925

Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
(Intercept)     -8.286327   0.856000  -9.680  < 2e-16 ***
male             0.506116   0.131991   3.834 0.000126 ***
age              0.064020   0.008135   7.869 3.56e-15 ***
education2      -0.210890   0.148310  -1.422 0.155038
education3      -0.120464   0.174595  -0.690 0.490220
education4      -0.082216   0.199469  -0.412 0.680212
currentSmoker    0.125147   0.187693   0.667 0.504921
cigsPerDay       0.016589   0.007482   2.217 0.026611 *
BPMeds           0.177341   0.282452   0.628 0.530094
prevalentStroke  1.158996   0.563826   2.056 0.039822 *
prevalentHyp     0.308709   0.166304   1.856 0.063412 .
diabetes        -0.318608   0.393231  -0.810 0.417807
totChol          0.003860   0.001334   2.894 0.003801 **
sysBP            0.011195   0.004451   2.515 0.011893 *
diaBP           -0.001726   0.007766  -0.222 0.824120
BMI              0.007535   0.015680   0.481 0.630828
heartRate       -0.007132   0.005136  -1.389 0.164946
glucose          0.009221   0.002748   3.356 0.000791 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 2176.6  on 2565  degrees of freedom
Residual deviance: 1918.2  on 2548  degrees of freedom
  (402 observations deleted due to missingness)
AIC: 1954.2

Number of Fisher Scoring iterations: 5
```

- Education as **categorical** variable

```
> framingham$education = factor(framingham$education)
> str(framingham)
'data.frame':   4240 obs. of  16 variables:
 $ male           : int  1 0 1 0 0 0 0 0 1 1 ...
 $ age            : int  39 46 48 61 46 43 63 45 52 43 ...
 $ education      : Factor w/ 4 levels "1","2","3","4": 4 2
1 3 3 2 1 2 1 1 ...
```

- car package gives the following (G)VIF figures

```
> car::vif(framinghamLog)
                    GVIF Df GVIF^(1/(2*Df))
male            1.268872  1        1.126442
age             1.302896  1        1.141445
education       1.121533  3        1.019300
```

- 👍 Use the **square** of the GVIF$^{\left(\frac{1}{2*df}\right)}$ value and apply the VIF rule of thumb

CSE 7302c

Case Study – Predicting Coronary Heart Disease (CHD)

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

Cohen’s Kappa, ROC Curve, Gains and Lift Charts

SOME MORE PERFORMANCE METRICS

Cohen's Kappa Metric

- Accuracy can often be a misleading metric when one category occurs more often than other in the given data-set. For example:
  - Occurrence of cancer in general population is 0.4%
  - If a prediction system blindly marks everyone as "No cancer", it will be 99.6% accurate

Cohen's Kappa Metric

- Kappa metric compares **Observed Accuracy** with **Expected Accuracy** (by random chance).

$$\boldsymbol{kappa} = \frac{\boldsymbol{Observed\ Accuracy - Expected\ Accuracy}}{\boldsymbol{1 - Expected\ Accuracy}}$$

$$Observed\ Accuracy = \frac{Correct\ Predictions\ (True\ Positives + True\ Negatives)}{Total}$$

Expected (Random chance) Accuracy uses Expected Frequencies, which are calculated the same way we did in Chi-Square calculation (Recall $Expected\ Frequency = \frac{Row\ Total * Column\ Total}{Grand\ Total}$)

Expected Frequencies are calculated only for the cells containing correct predictions.

Cohen's Kappa Metric

- Total= 30+357+9+2170=2566
- **Observed Accuracy**=(30+2170)/2566=0.857

- Expected True Positives=(387*39)/2566 = 5.88
- Expected True Negatives=(2179*2527)/2566 = 2145.88
- **Expected Accuracy by random chance**=(5.88+2145.88)/2566 = 0.839

$$kappa = \frac{Observed\ Accuracy - Expected\ Accuracy}{1 - Expected\ Accuracy} = \frac{0.857 - 0.839}{1 - 0.839} = \frac{0.018}{0.161} = 0.11$$

Slightly better than random chance!

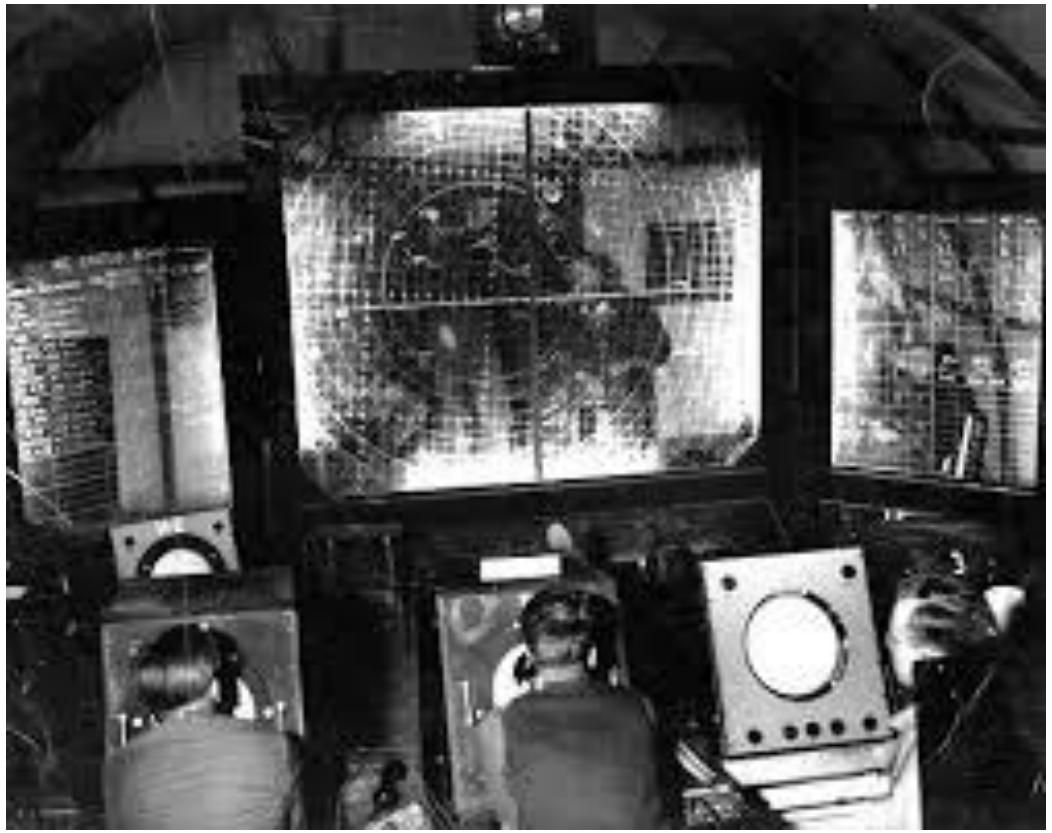
10-year CHD risk		Predicted	
		True	False
Actual	True	30	357
	False	9	2170

Kappa Value	Interpretation*
<0	No agreement
0-0.2	Slight
0.21 to 0.4	Fair
0.4 to 0.6	Moderate
0.6 to 0.8	Substantial
0.8 to 1	Almost Perfect

* Landis, J.R.; Koch, G.G. (1977). "The measurement of observer agreement for categorical data". *Biometrics* **33** (1): 159–174

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	13	6	916	157
0.3	45	80	842	125
0.1	139	473	449	31

- Actual Counts
  - Without CHD: 922
  - With CHD: 170

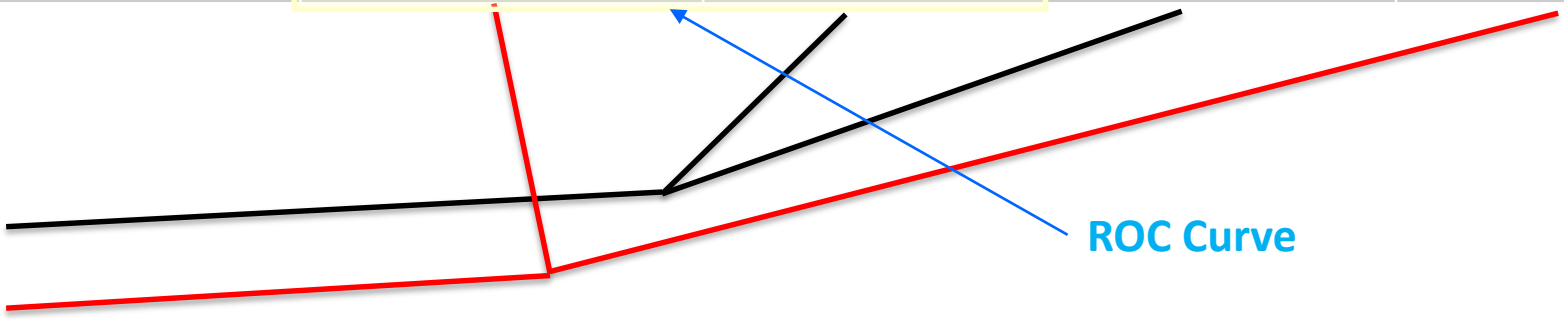
```
> table(test$TenYearCHD, predictTest > 0.5)

   FALSE TRUE
0    916    6
1    157   13
```

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	13/170	6/922	916/922	157/170
0.3	45/170	80/922	842/922	125/170
0.1	139/170	473/922	449/922	31/170

- Actual Counts
  - Without CHD: 922
  - With CHD: 170



ROC Curves and AUC

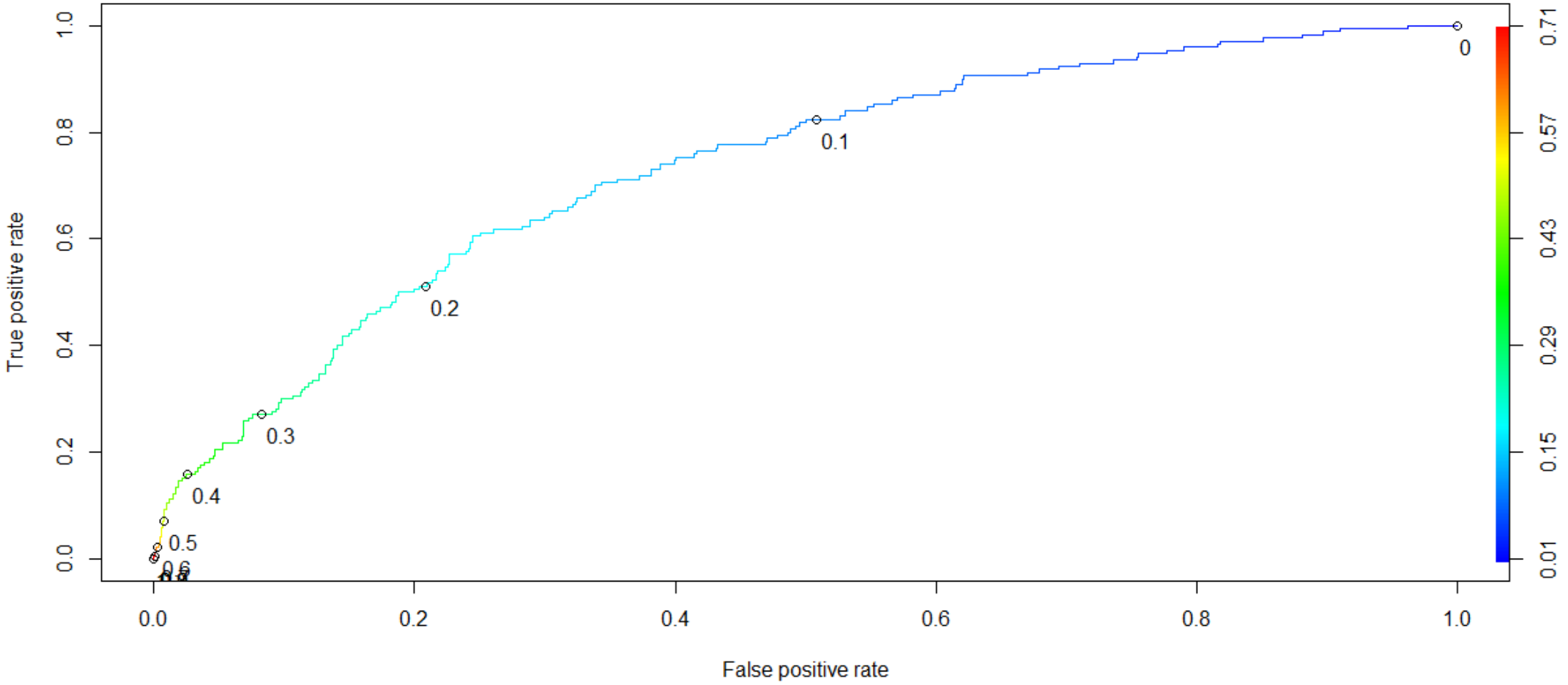
- ROC – Plot of True Positive Rate vs False Positive Rate, i.e., Sensitivity vs 1-Specificity

Probability Threshold for Discriminating Between High Risk and Low Risk of Having Ten Year CHD	Sensitivity: True Positive Rate	False Positive Rate
0.9	0/170	0/922
0.7	1/170	1/922
0.5	13/170	6/922
0.3	45/170	80/922
0.1	139/170	473/922

P(Predicting CHD | Have CHD) P(Predicting CHD | Do Not Have CHD) ROC Curve

ROC Curves and AUC

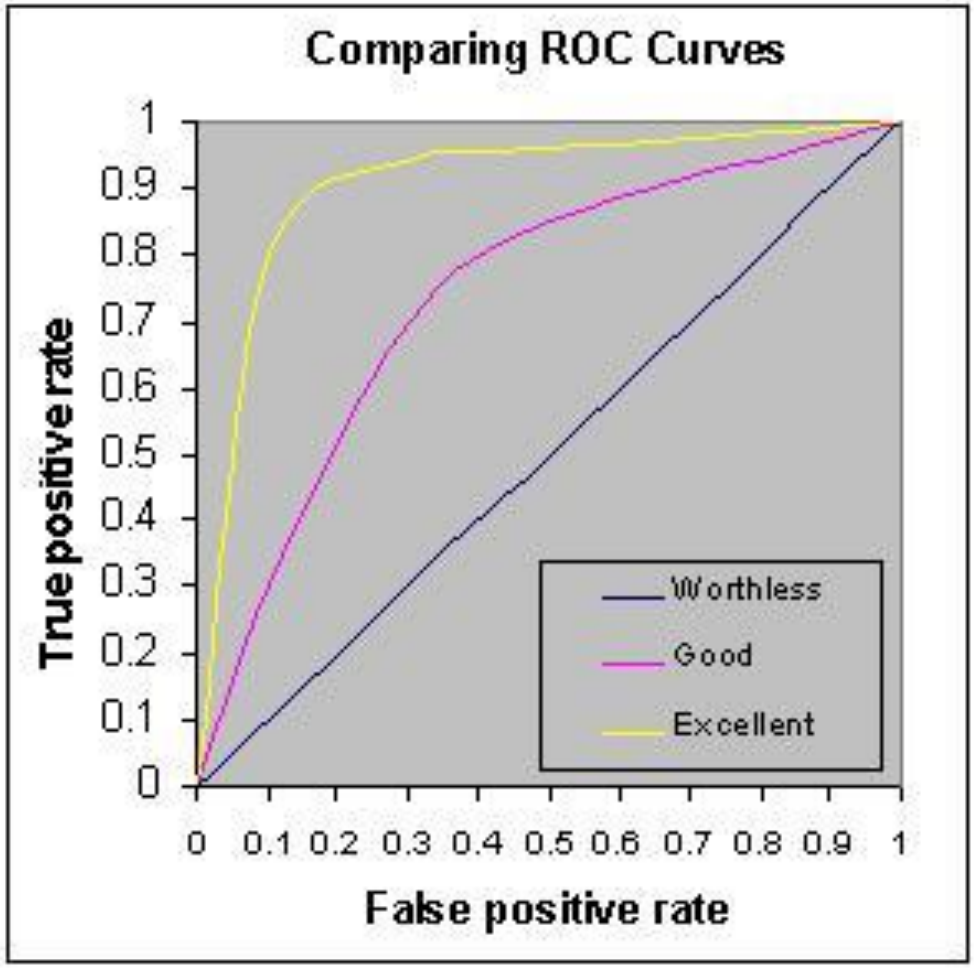
- ROC – Plot of True Positive Rate vs False Positive Rate, i.e., Sensitivity vs 1-Specificity



ROC Curves and AUC

- AUC – Measures discrimination, i.e., ability to correctly classify those with and without CHD.
- If you randomly pick one person who HAS CHD and one 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.

ROC Curves and AUC



Rough rule of thumb:

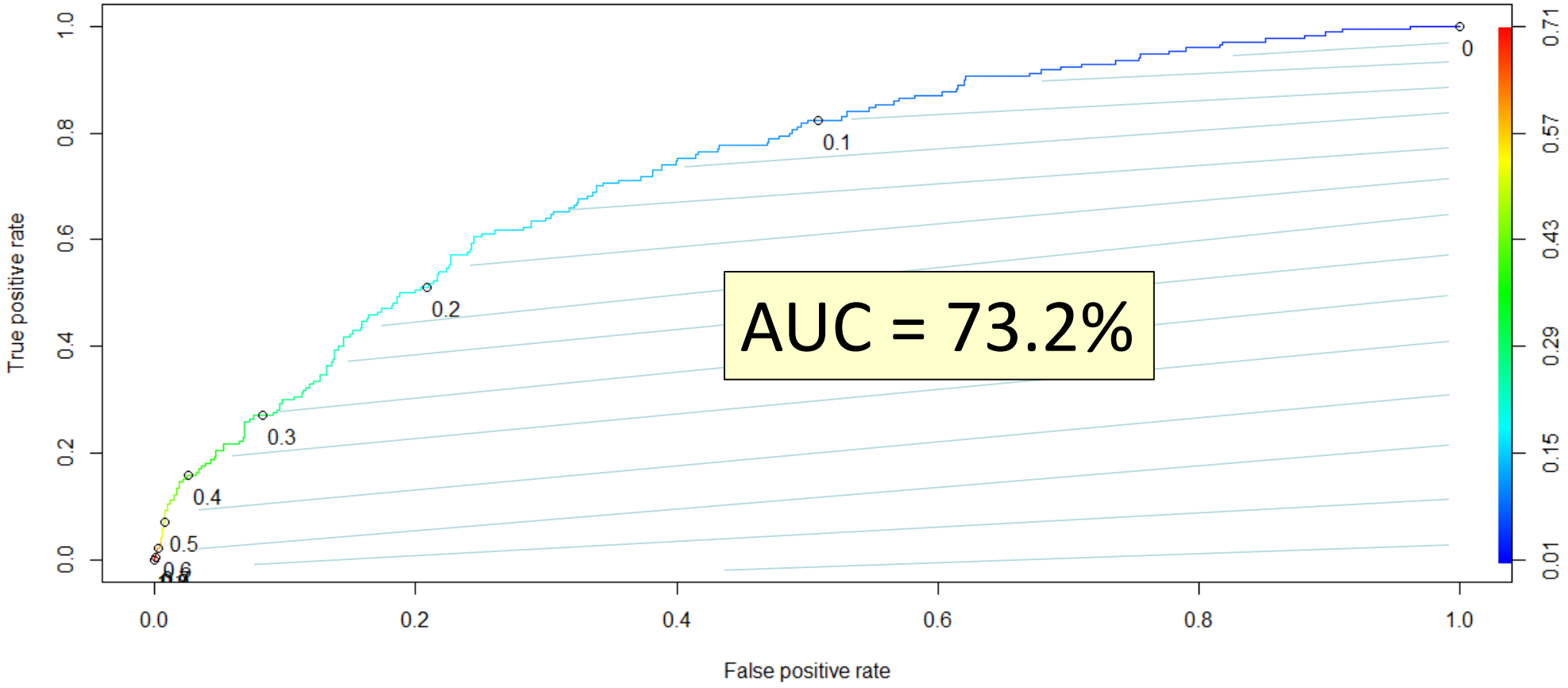
- 0.90 -1.0 = Excellent
- 0.80 – 0.90 = Good
- 0.70 – 0.80 = Fair
- 0.60 – 0.70 = Poor
- 0.50 – 0.60 = Fail

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

ROC Curves and AUC

BREAK

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



Gains and Lift Charts

- 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.
  - In credit risk modelling, you might want to target only certain customers for offering a new loan product.

- **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).

Gains and Lift Charts

- 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.

Gains and Lift Charts

- 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

Gains and Lift Charts

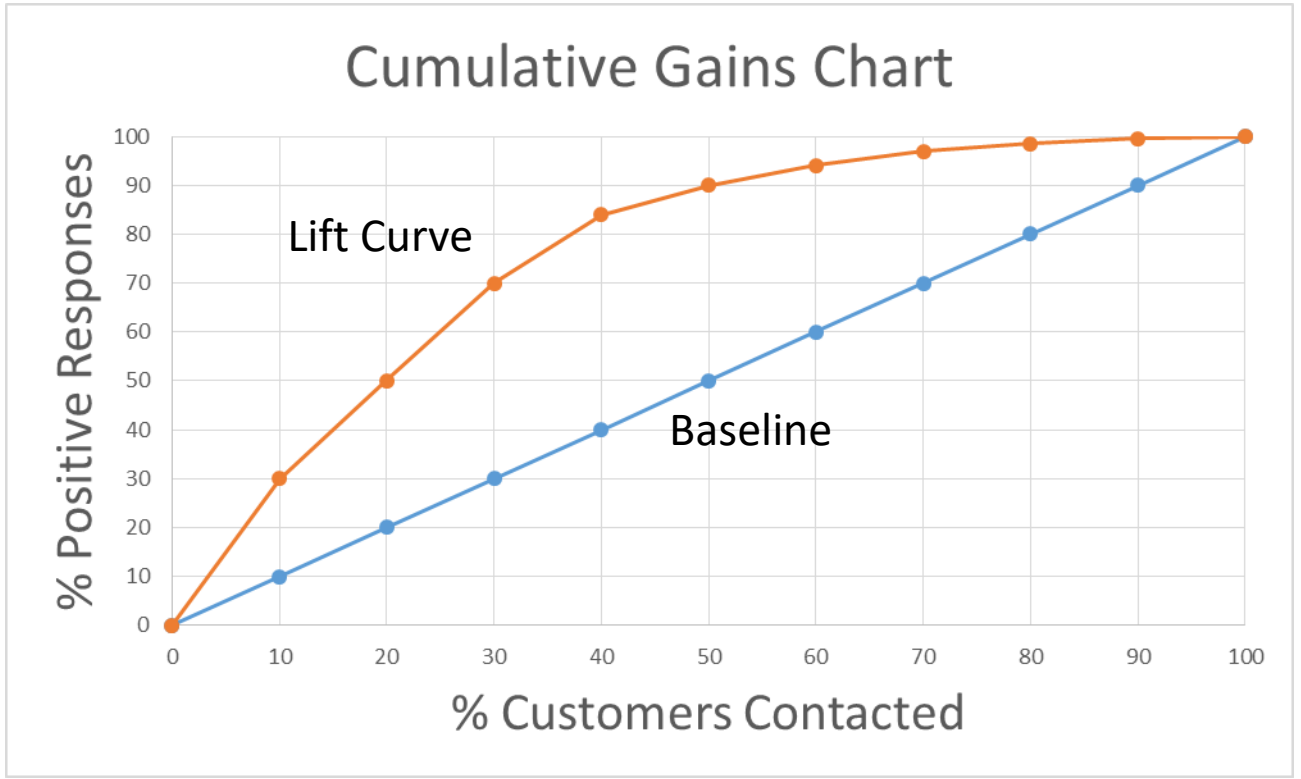
- With a predictive model, where the model assigns a probability to each customer, the customers are ordered and divided into deciles (or any other quantiles). They are then called in decreasing order of probability to buy.

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

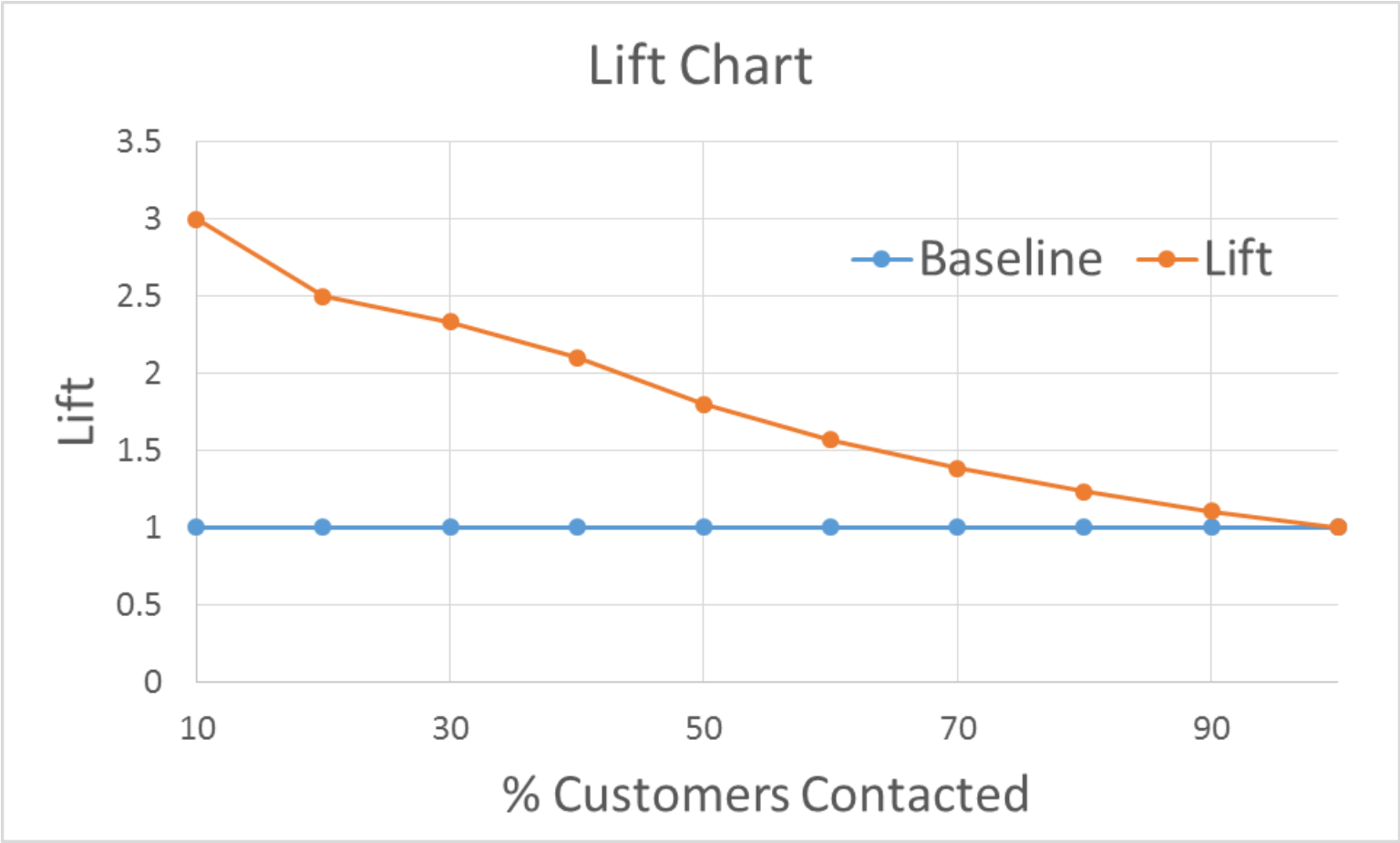
Gains and Lift Charts

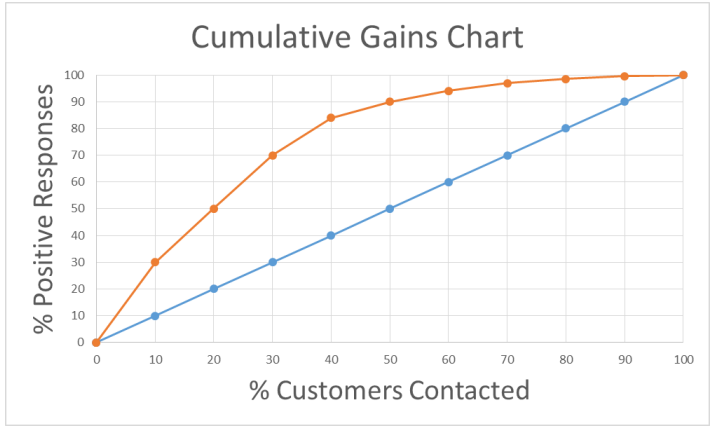
% Called	Called at Random	Called According to Model Score
0	0	0
10	10	30
20	20	50
30	30	70
40	40	84
50	50	90
60	60	94
70	70	97
80	80	98.5
90	90	99.5
100	100	100

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



Gains and Lift Charts





- 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.

Evaluating Model Accuracy or Performance

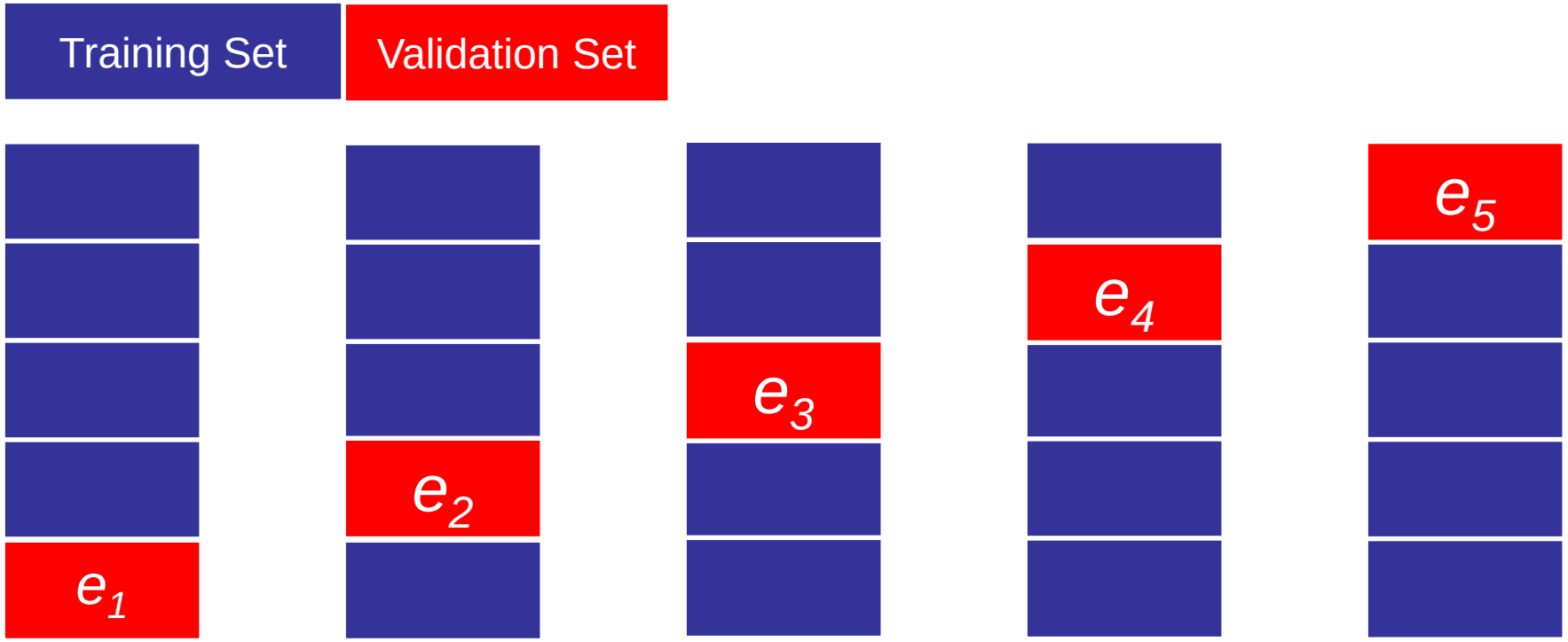
BIAS-VARIANCE TRADEOFF

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 and 10.



Calculate **Mean** and **Standard Deviation** of the *k* errors.

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^2
  - AIC

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.

Bias-Variance Tradeoff

- 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-Variance Tradeoff

- 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.

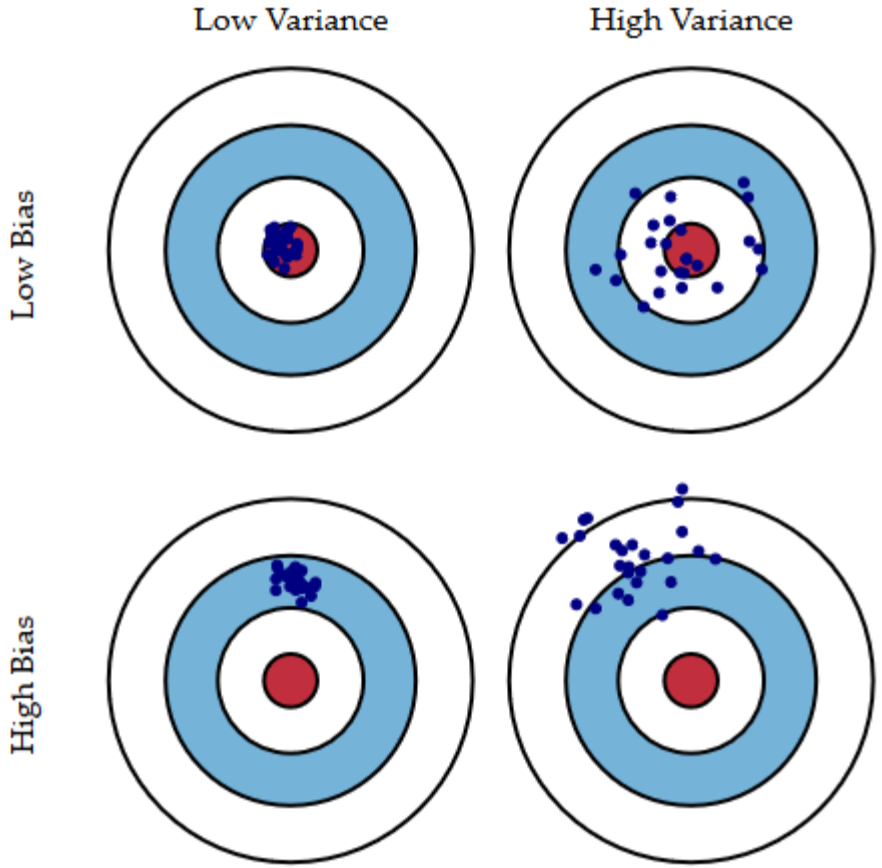
- Variance arises due to the model being overly sensitive to small fluctuations in the training data. Such a model ***overfits*** the data, including the random noise rather than just the actual behaviour.

Bias-Variance Tradeoff

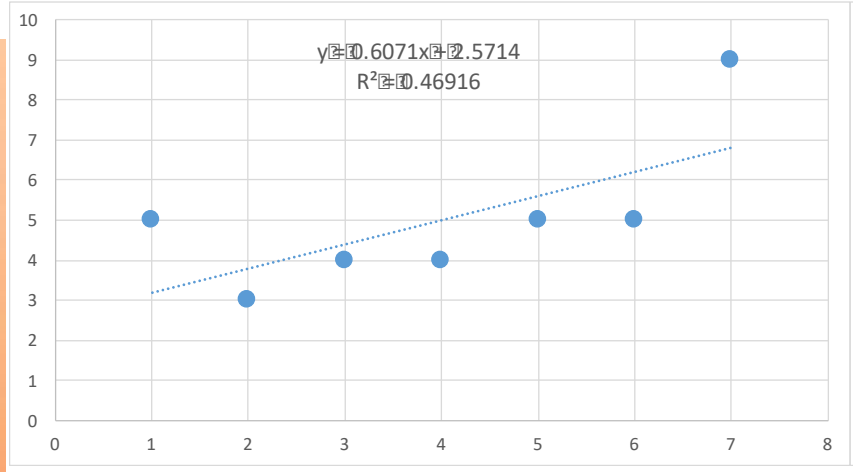
- An ideal model will **both** *capture the patterns* in the training data **and** *generalize* well enough to the unseen (testing) data.
- Unfortunately, it is generally impossible to do both and hence the tradeoff.
- All supervised models (classification, regression, etc.) are affected by this.

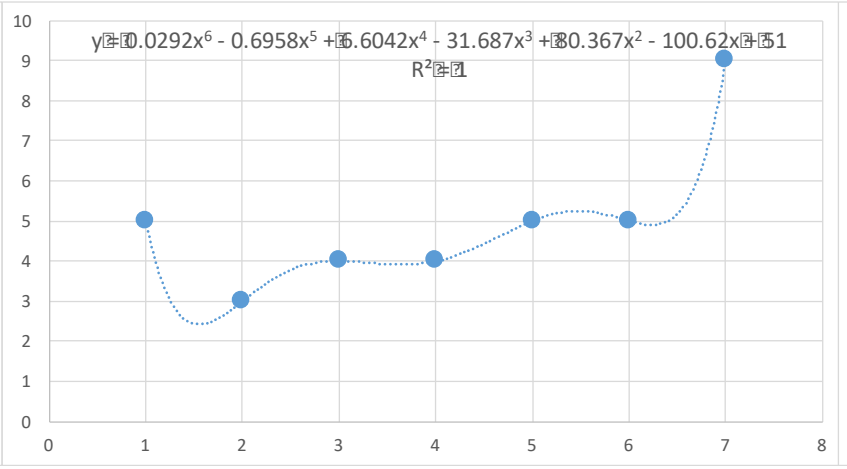
Bias-Variance Tradeoff

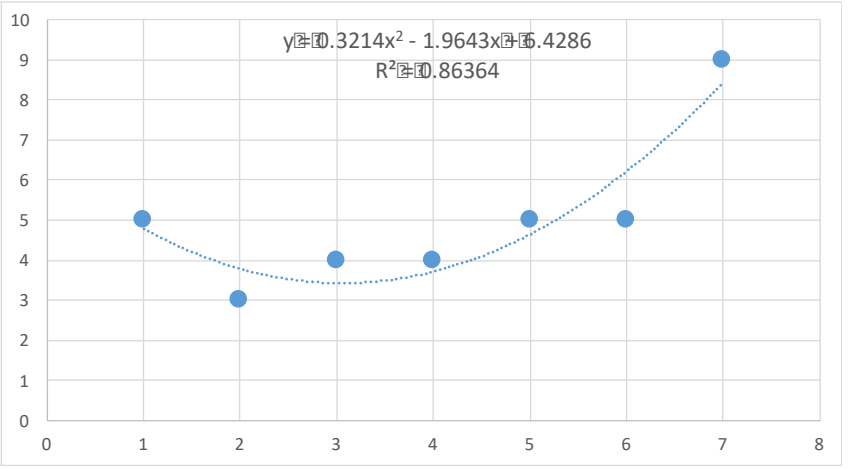
- Bulls-eye is a model that correctly predicts the real values.
- Each hit is a model based on chance variability in training datasets.



Bias-Variance Tradeoff and Underfitting vs Overfitting







Too Simple a Model Underfit	Too Complex a Model Overfit	Right Model Reasonable fit

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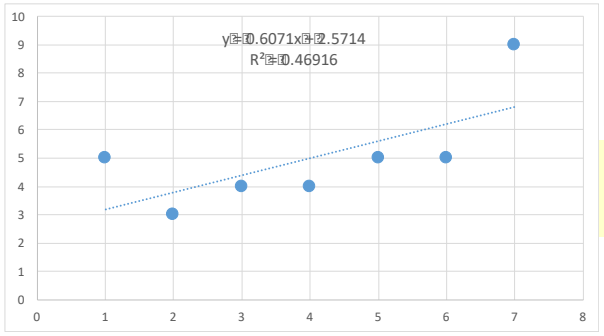
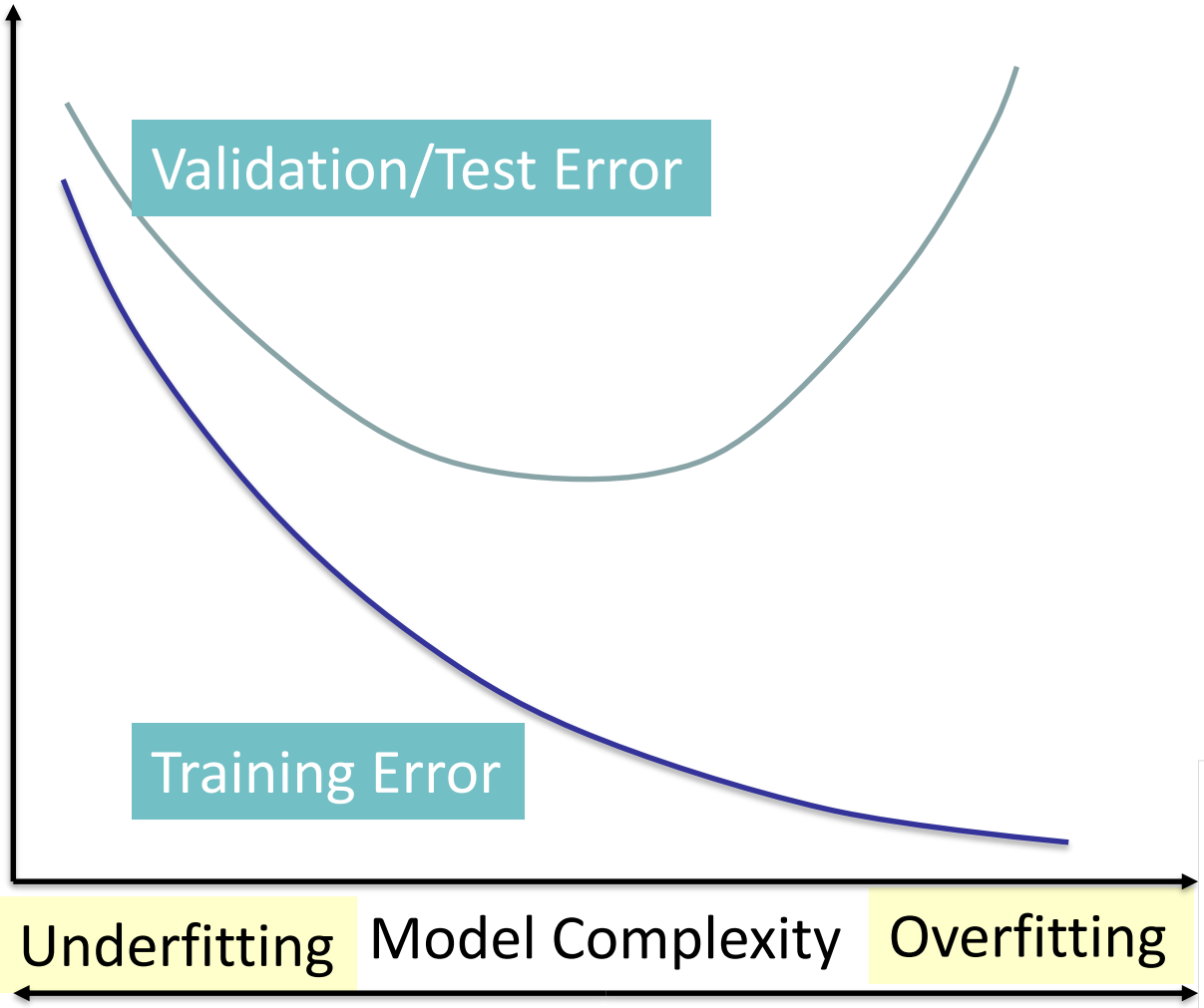
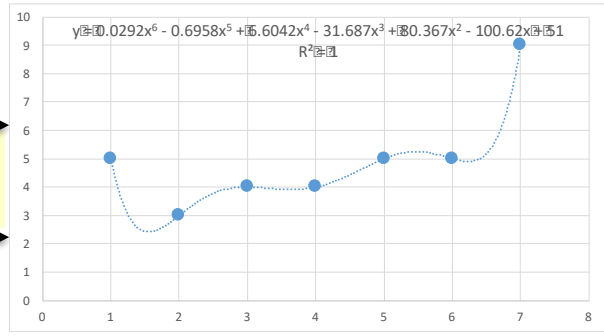
Bias-Variance Tradeoff and Underfitting vs Overfitting







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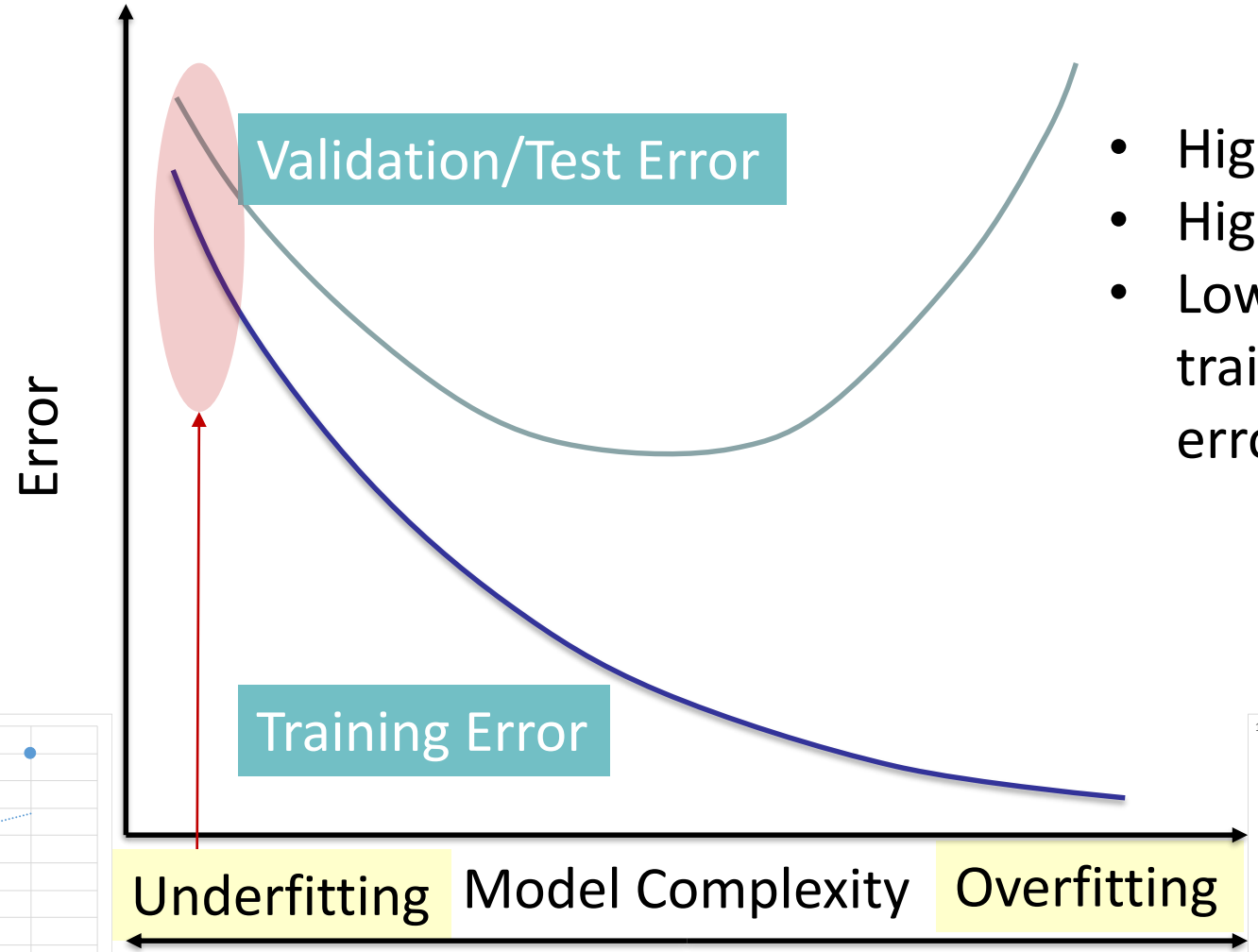
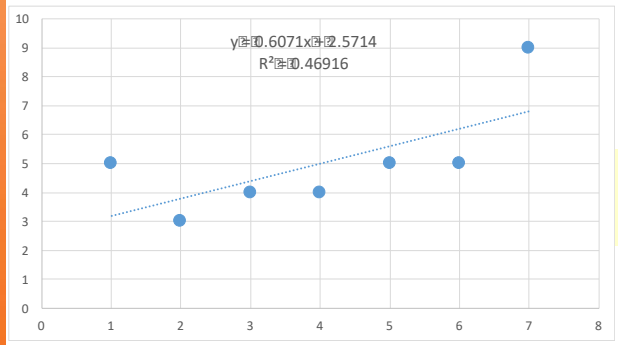
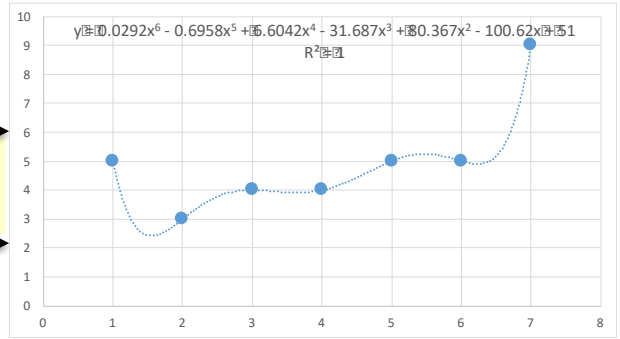
Diagnosing Bias and Variance



Underfitting (Bias)

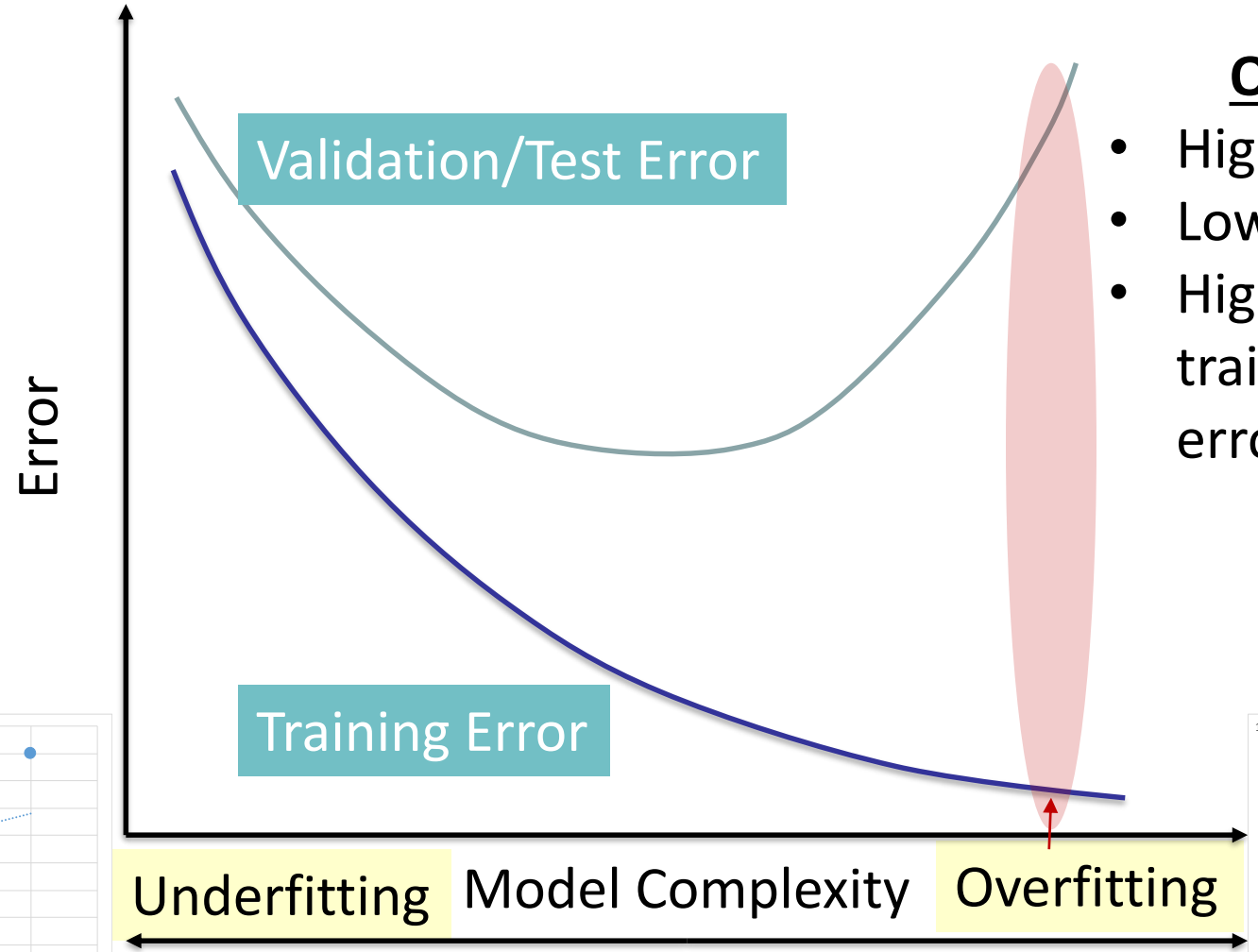
- High Bias problem
- High training error
- Low difference between training and test/validation errors





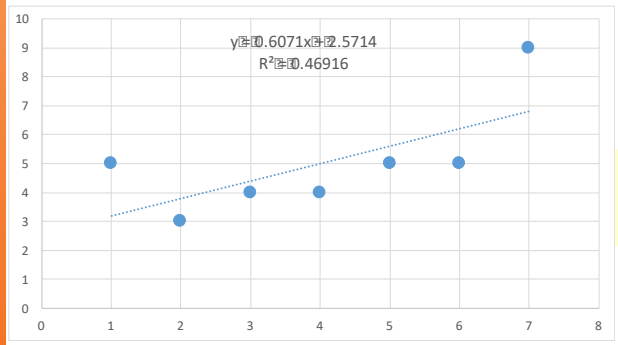
CSE 73026

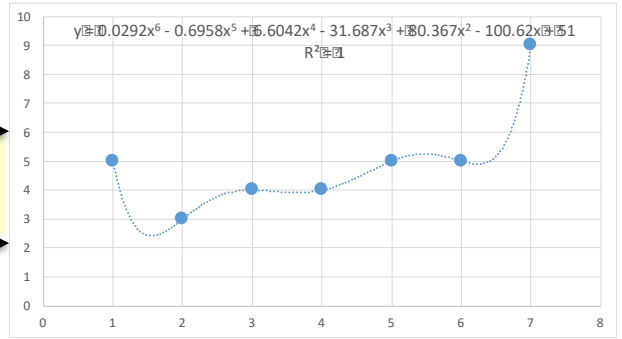
Diagnosing Bias and Variance



Overfitting (Variance)

- High Variance problem
- Low training error
- High difference between training and test/validation errors





CSE 73026

Bias-Variance Tradeoff

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.

Bias-Variance Tradeoff

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 layers.
- 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

Bias-Variance Tradeoff

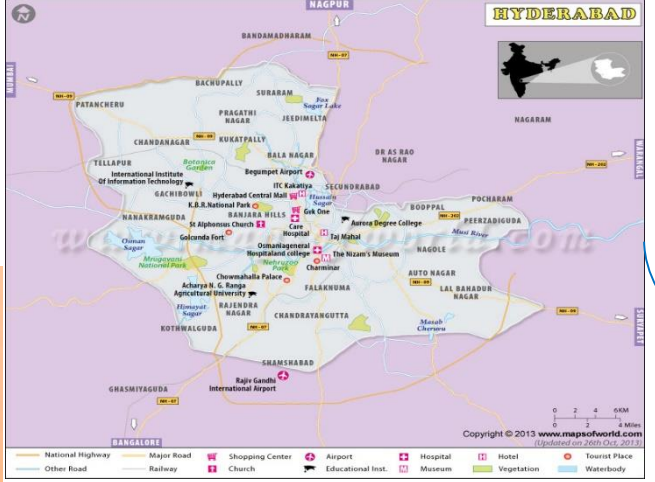
Ways of detecting and minimizing Bias and Variance

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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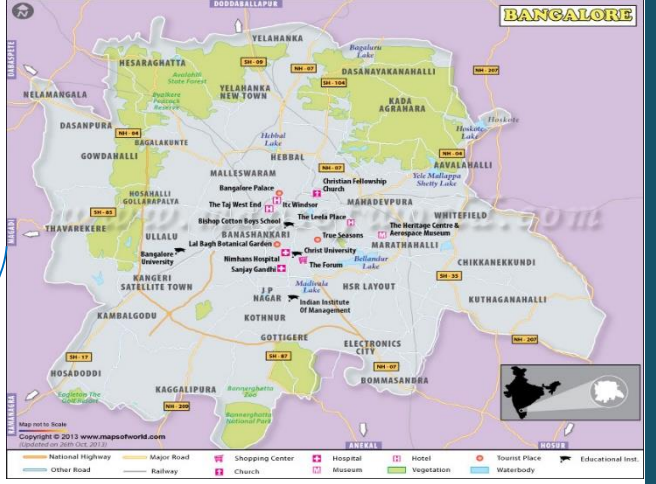

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+91-9618483483 (Corporates)

BENGALURU

Floors 1-3, L77, 15th Cross Road, 3A Main Road, Sector 6, HSR Layout, Bengaluru – 560 102
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