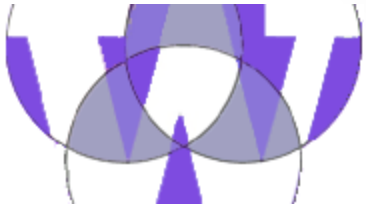
Introduction to Data Science

Lecture 09; May 21st, 2018

Ernst Henle
ErnstHe@UW.edu
Skype: ernst-henle

Agenda



- 18:00-18:05 Announcements
  - 4 Quizzes: 2 in class and 2 for homework
  - LinkedIn: start a discussion or comment on an existing discussion
  - Applebee's: 9:15 today; 13856 Bel Red Road ; (140th Ave)
- 18:05-18:25 Overfitting and Confusion Matrix
- 18:25-18:40 Lesson 09 Quiz 0a Confusion Matrix
- 18:40-19:05 ROC Chart Intro
- 18:55-19:05 Break
- 19:05-19:15 Lesson 09 Quiz 0b ROC Intro
- 19:25-19:45 How to make an ROC
- 19:45-19:55 Break
- 19:55-20:30 Lesson_09
- 20:30-21:00 L09-AccuracyMeasures.py
- Predictive Analytics Iteration Trap (Time Permitting)

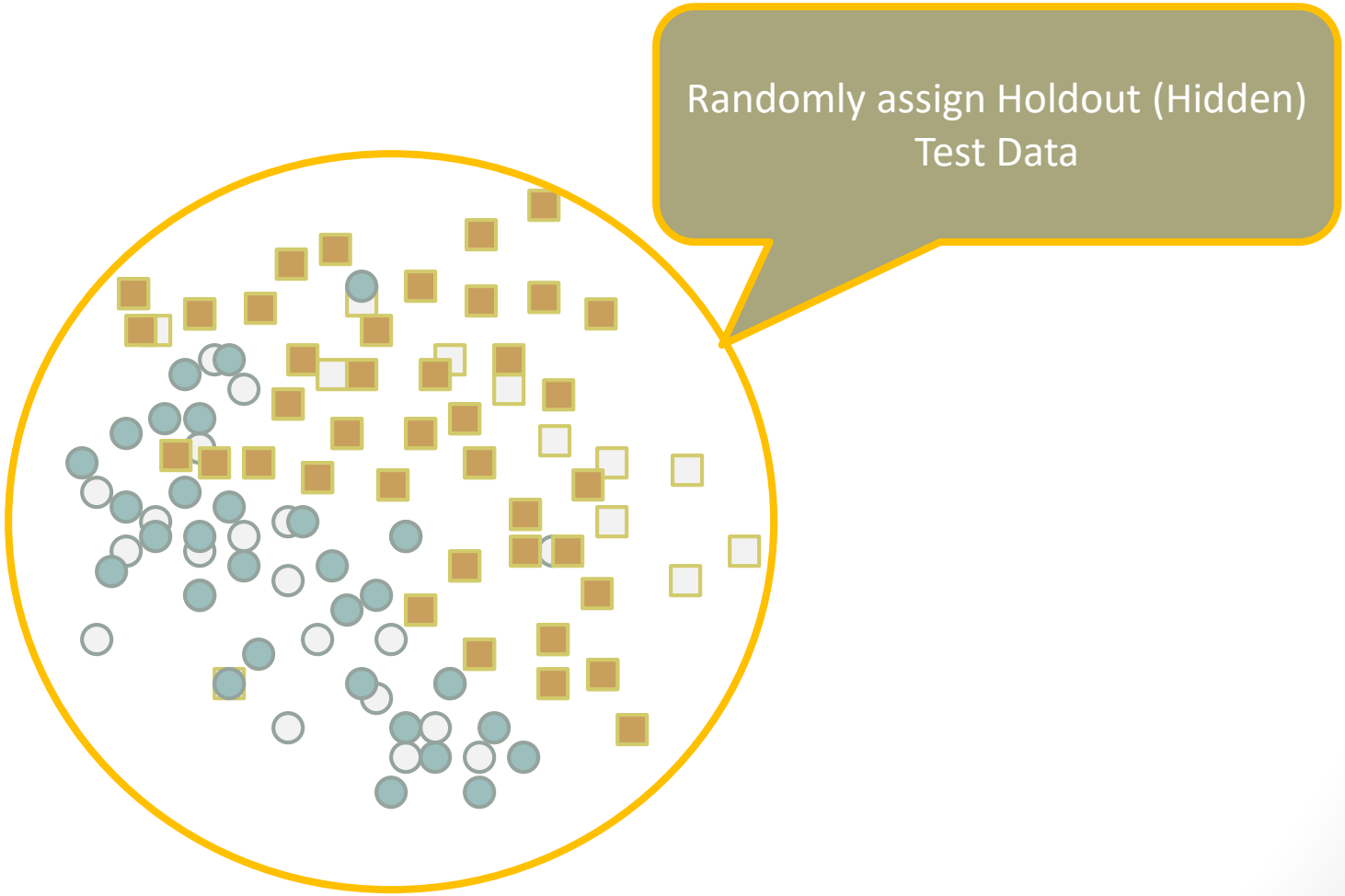
Over-fitting and Confusion Matrix

Evaluate Model

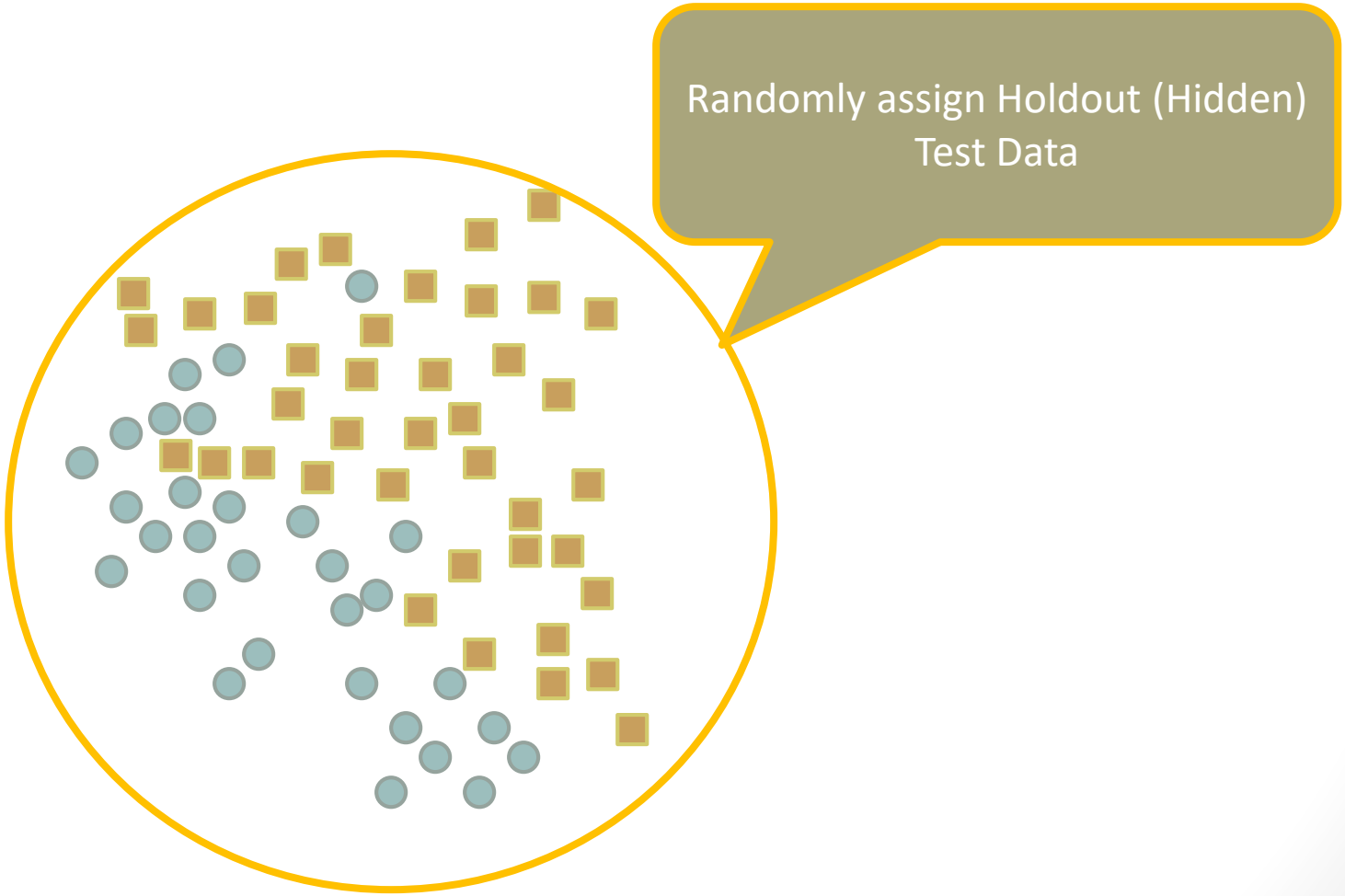
- The following segment will use an over-fitting example to explain the following concepts:
  - Modeling Data
    - Training Data
    - Test Data
  - Model (Hypothesis)
  - Over-fitting
  - Model Accuracy
  - Confusion Matrix (Classification Matrix)
    - True Positive
    - False Positive
    - True Negative
    - False Negative

Evaluate Model: All Data

Evaluate Model: Test Data

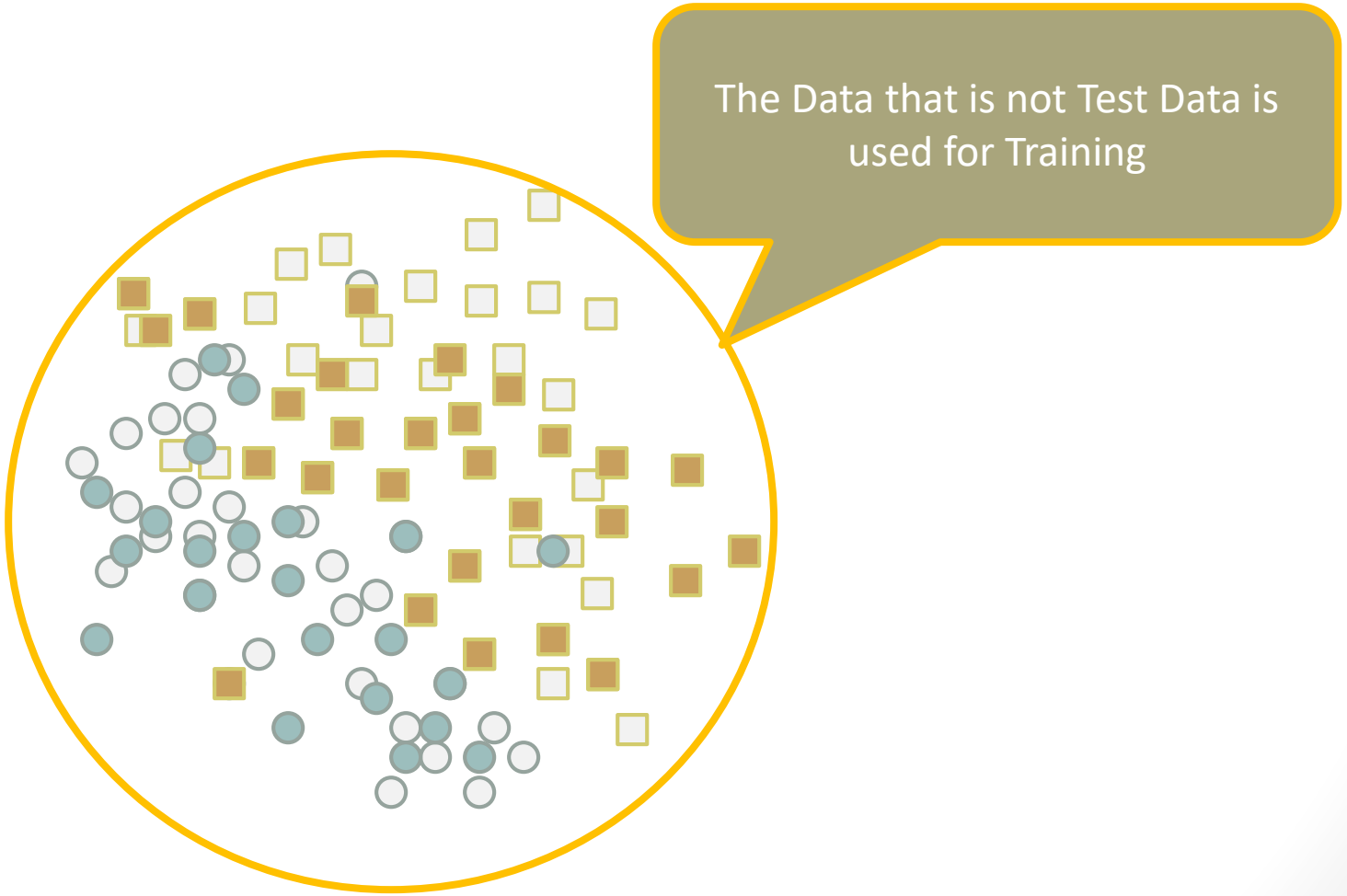


Evaluate Model: Test Data

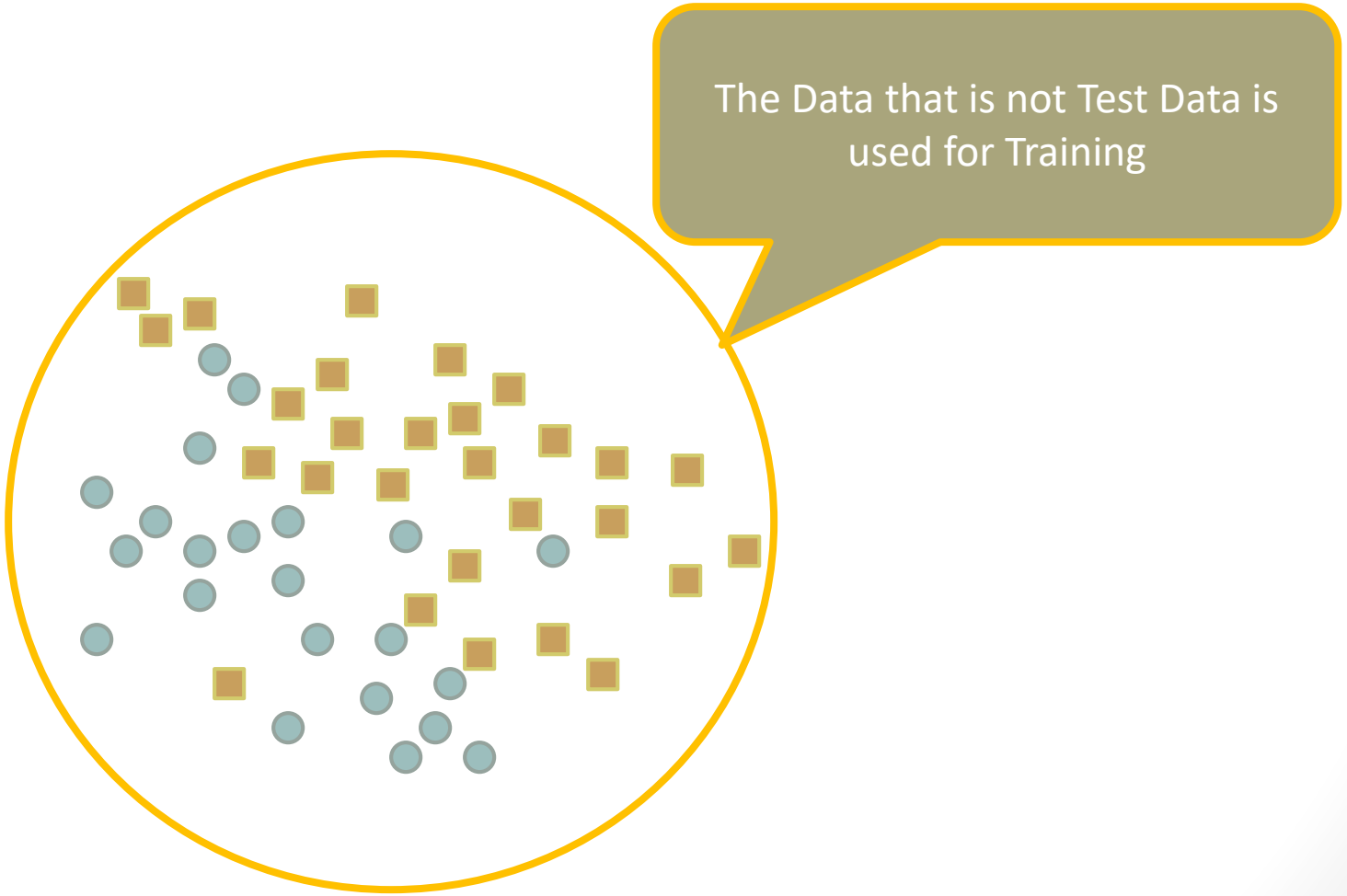


Evaluate Model: All Data

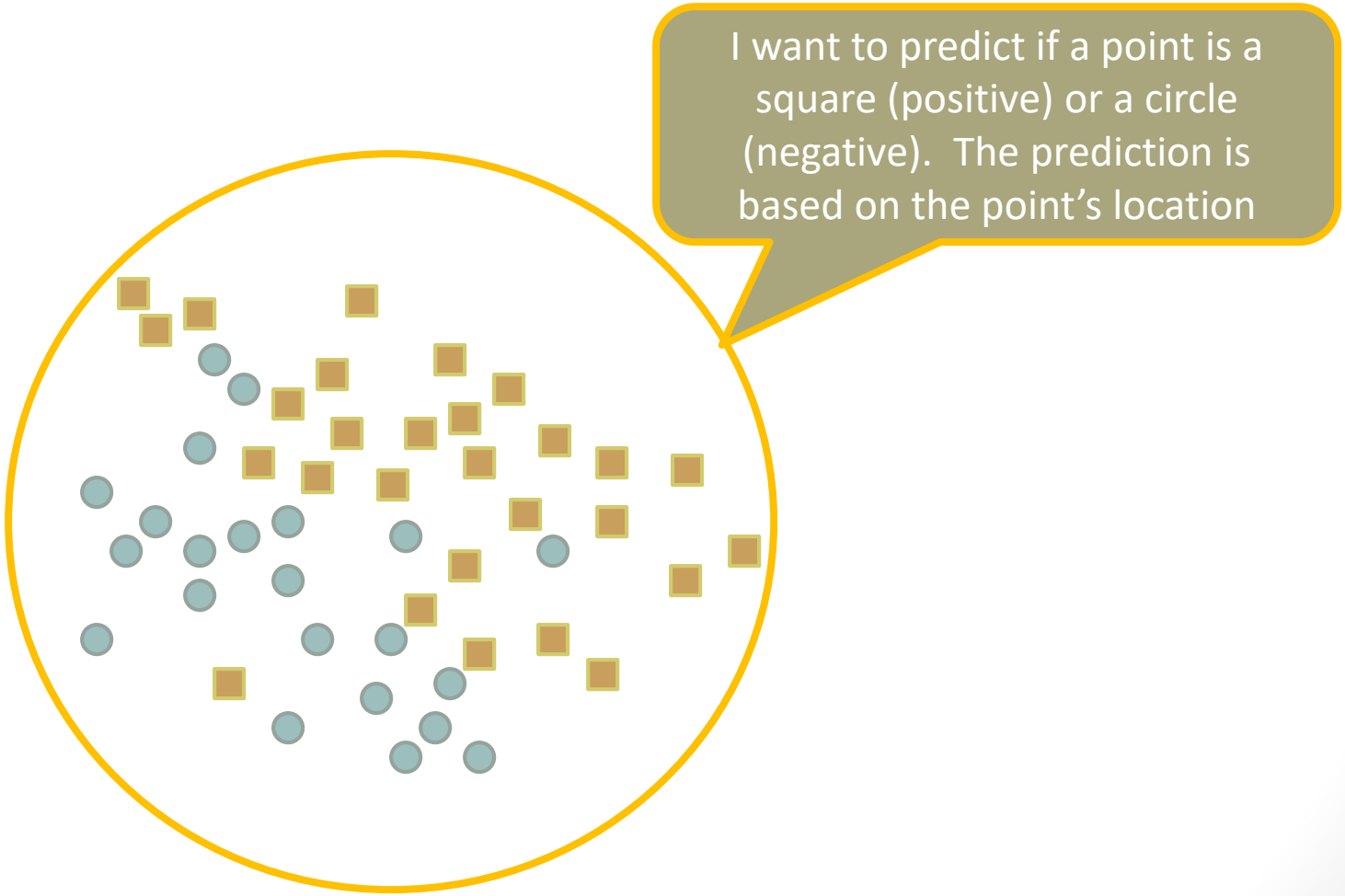
Evaluate Model: Training Data



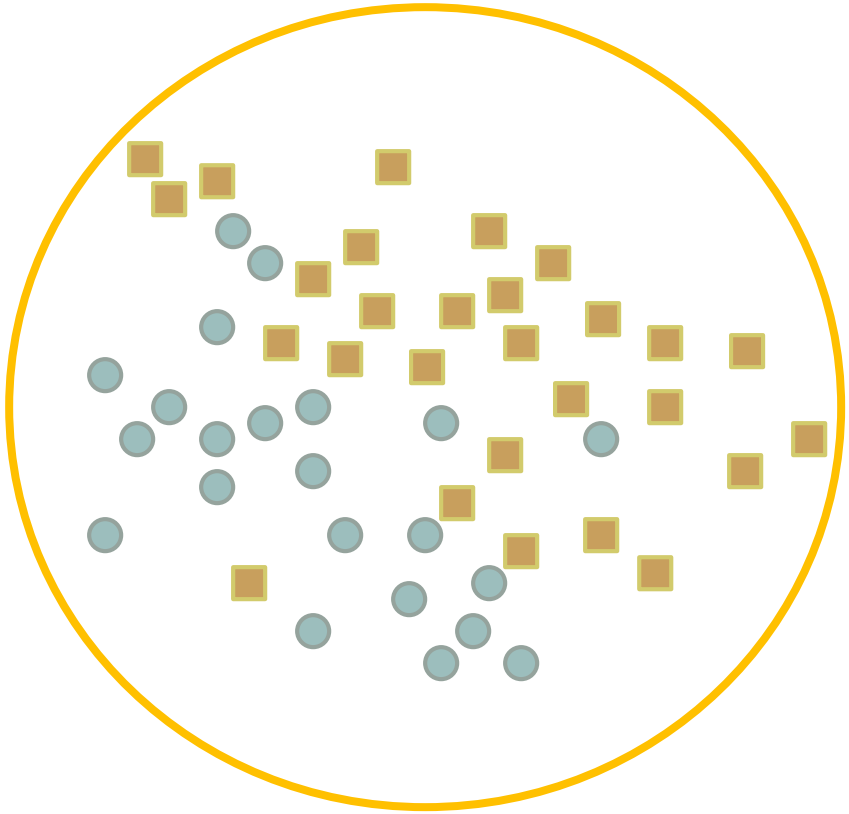
Evaluate Model: Training Data



Evaluate Model: Training



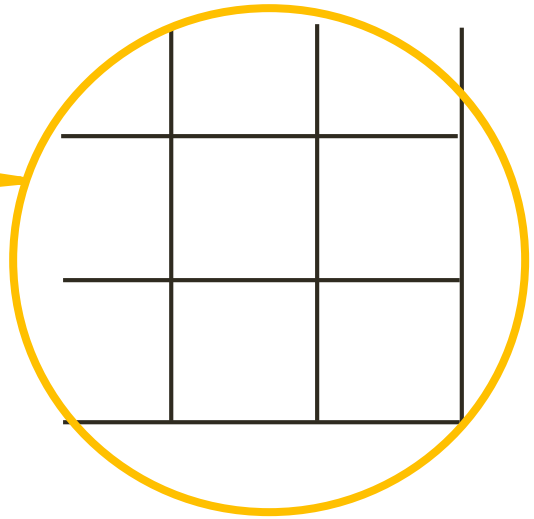
Evaluate Model: Training

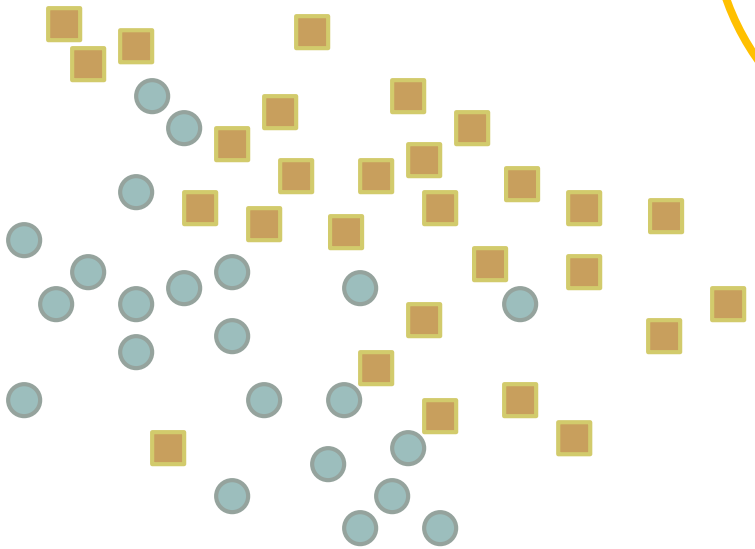


isSquare ~ xLocation + yLocation

Evaluate Model: Confusion Matrix

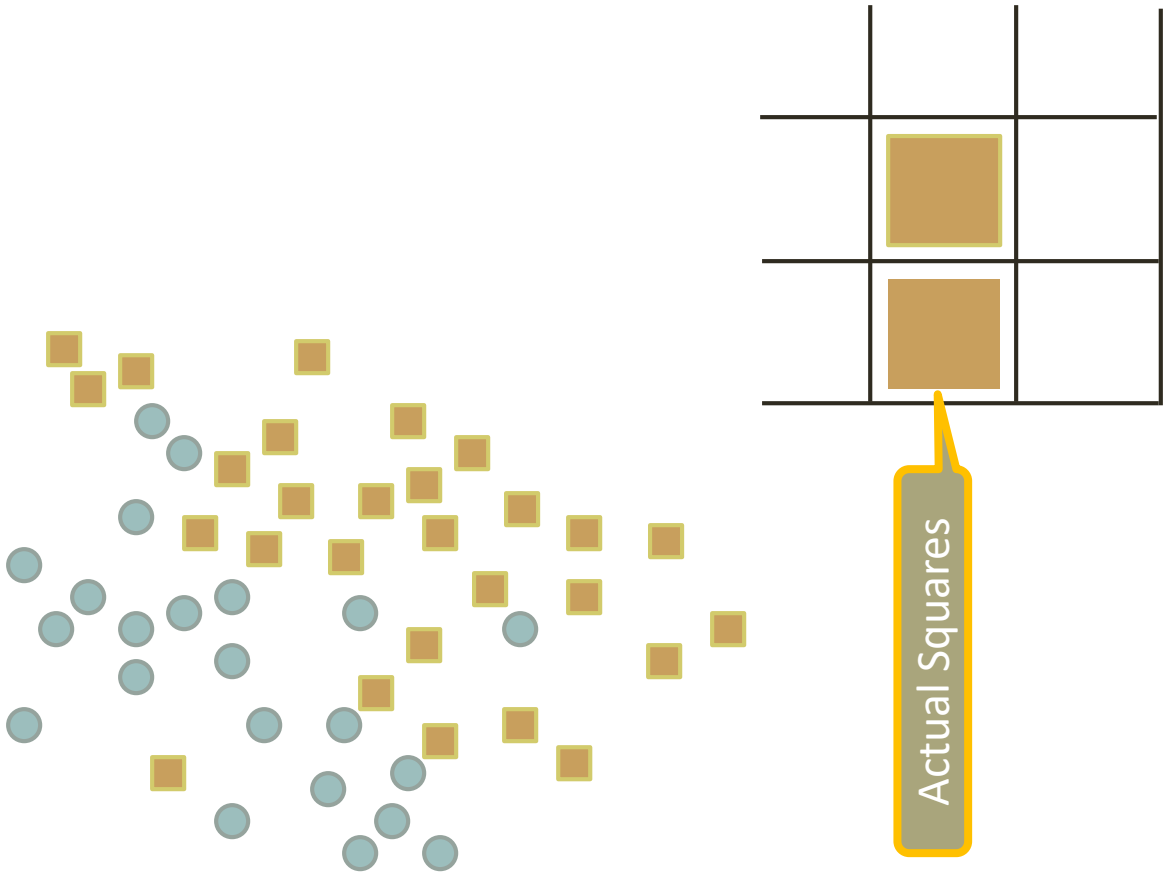
Confusion Matrix (Classification Matrix): Compare Squares and Circles with Predicted Squares and Circles





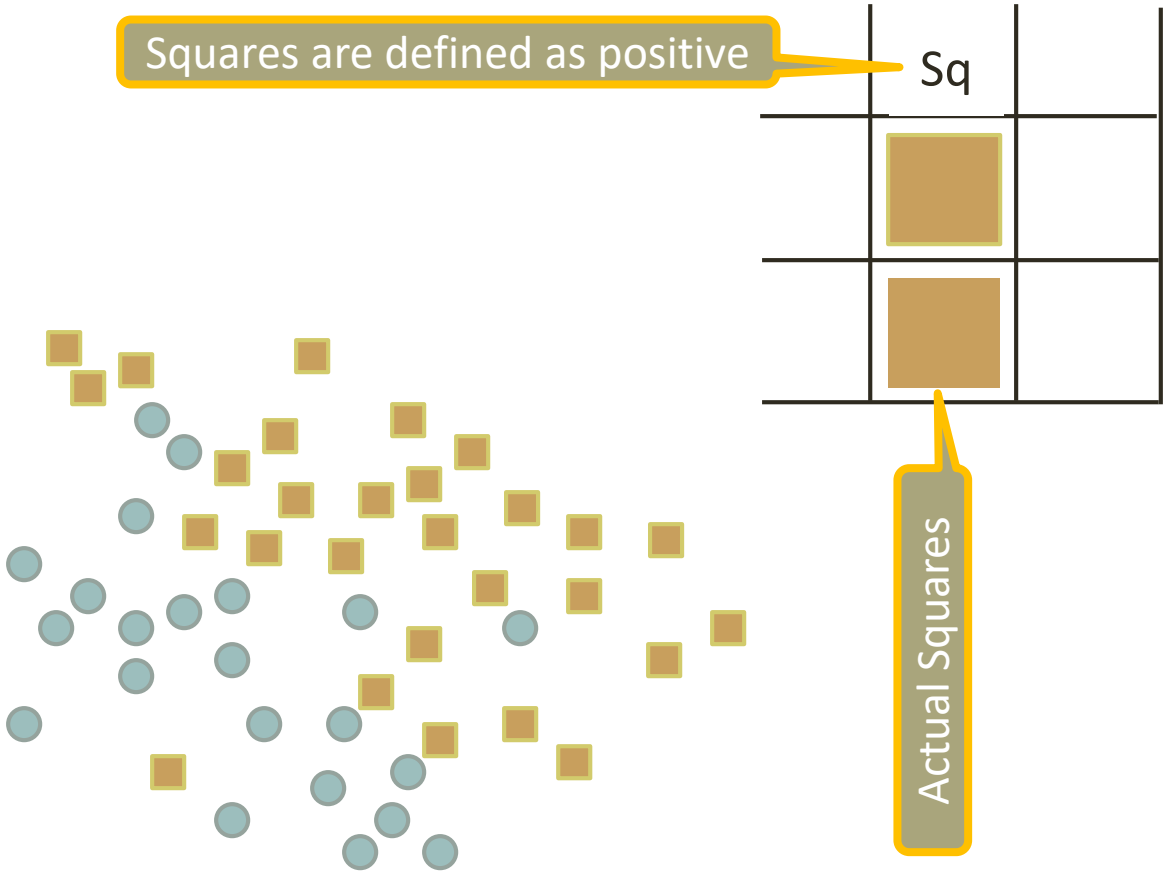
isSquare ~ xLocation + yLocation

Evaluate Model: Confusion Matrix



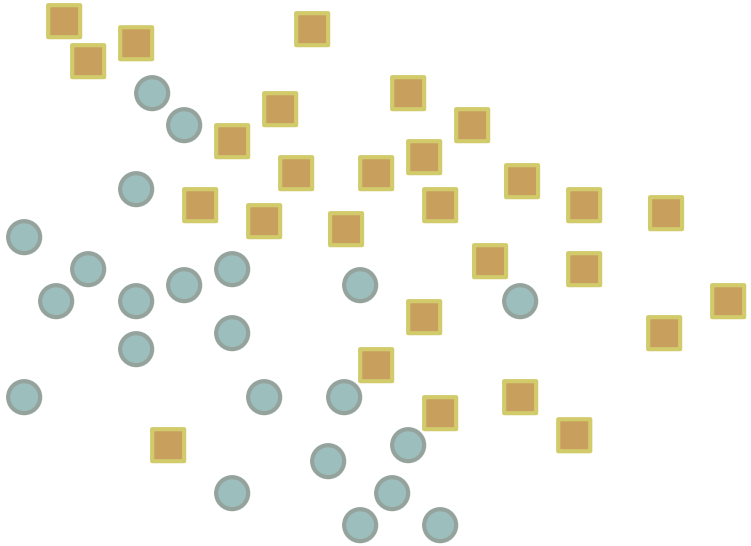
isSquare ~ xLocation + yLocation

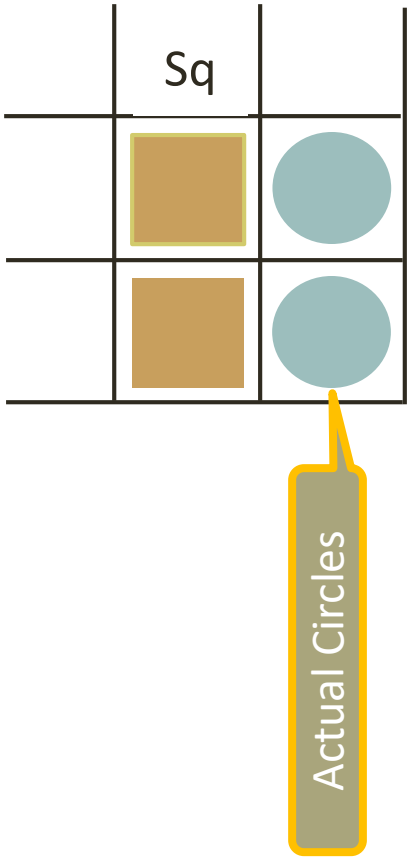
Evaluate Model: Confusion Matrix



isSquare ~ xLocation + yLocation

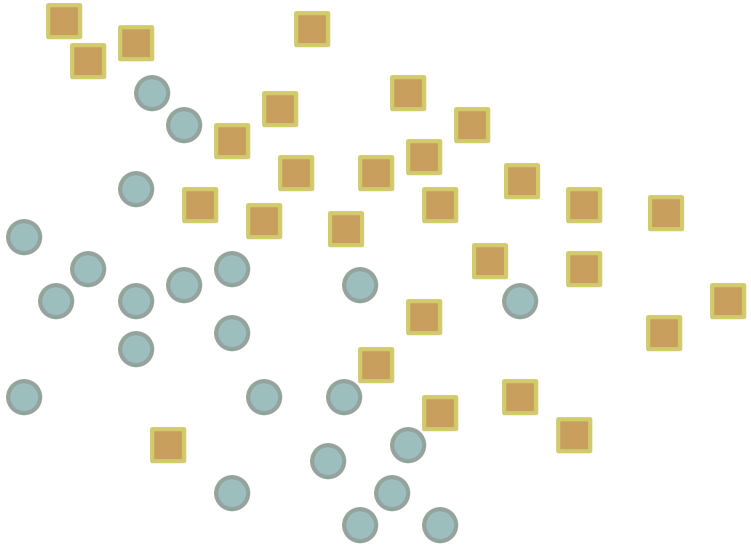
Evaluate Model: Confusion Matrix





isSquare ~ xLocation + yLocation

Evaluate Model: Confusion Matrix



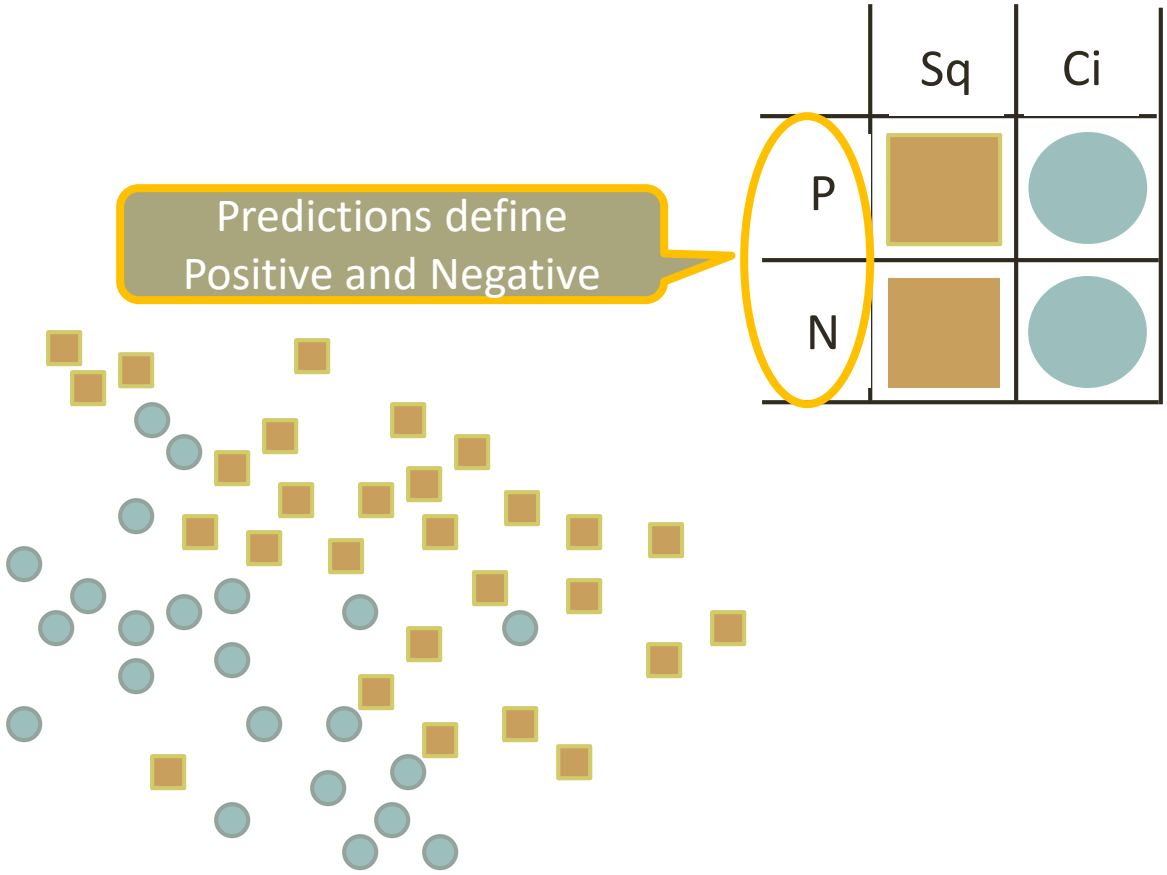
Circles are defined as negative

	Sq	Ci

Actual Circles

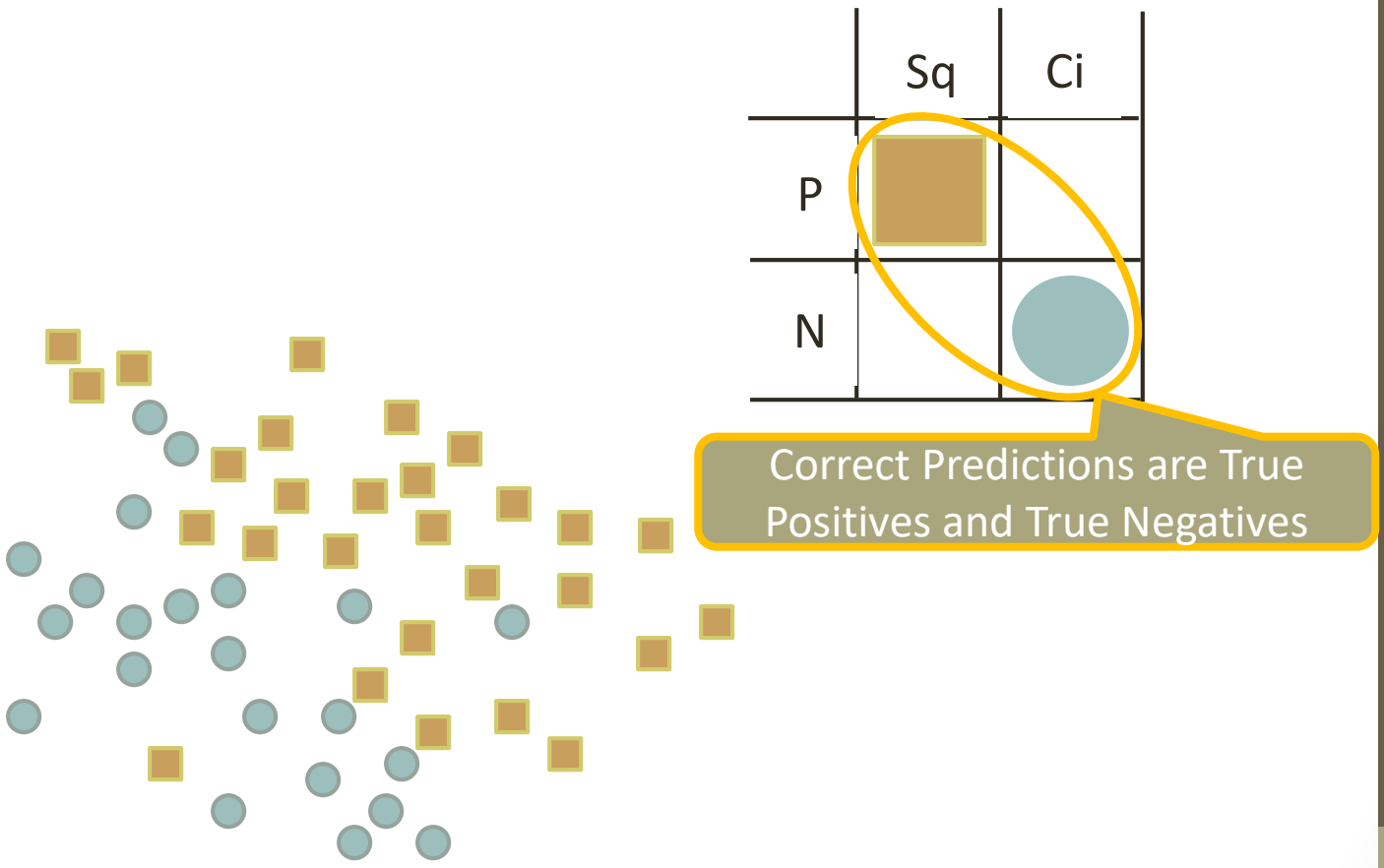
isSquare ~ xLocation + yLocation

Evaluate Model: Confusion Matrix



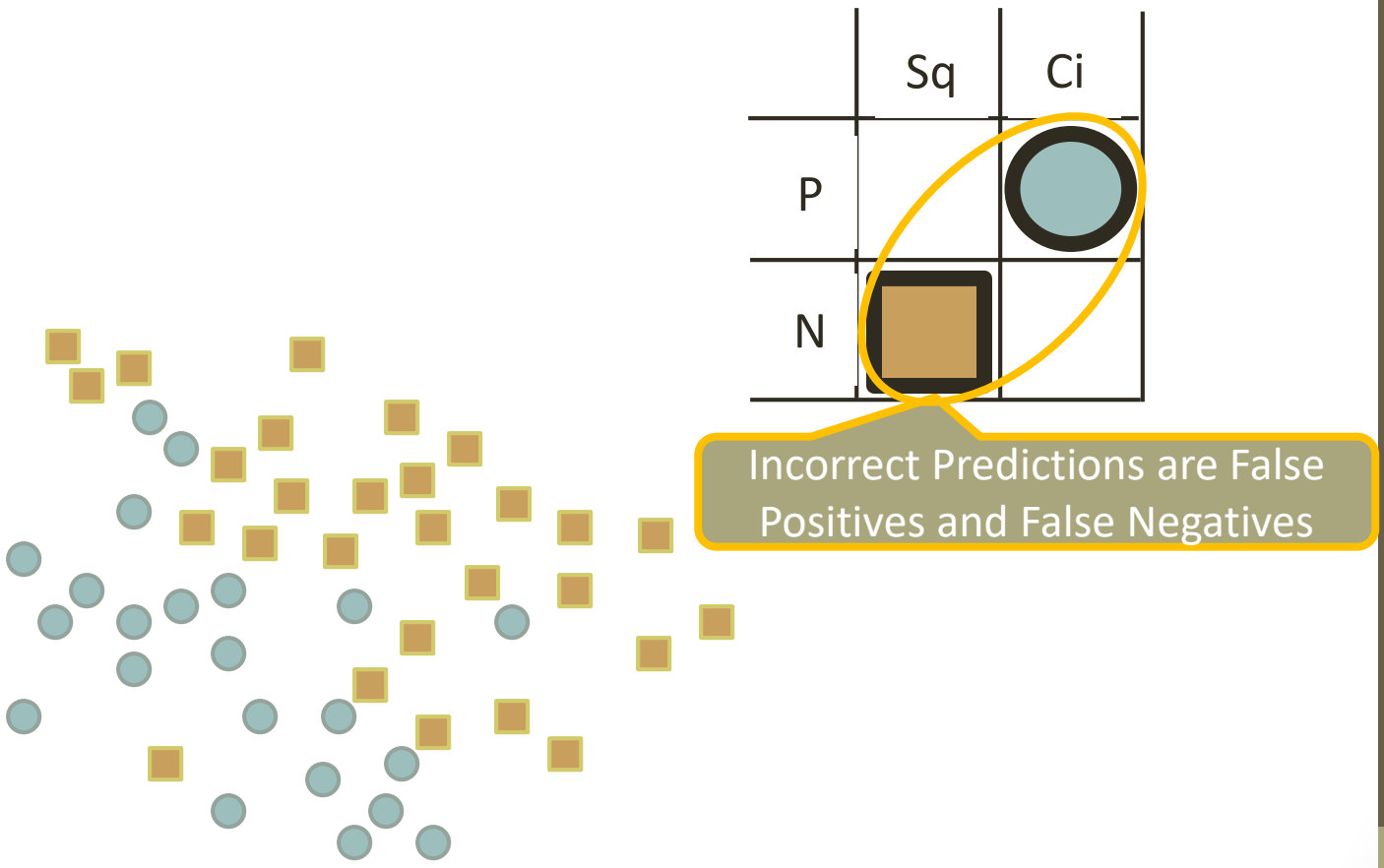
isSquare ~ xLocation + yLocation

Evaluate Model: Confusion Matrix



isSquare ~ xLocation + yLocation

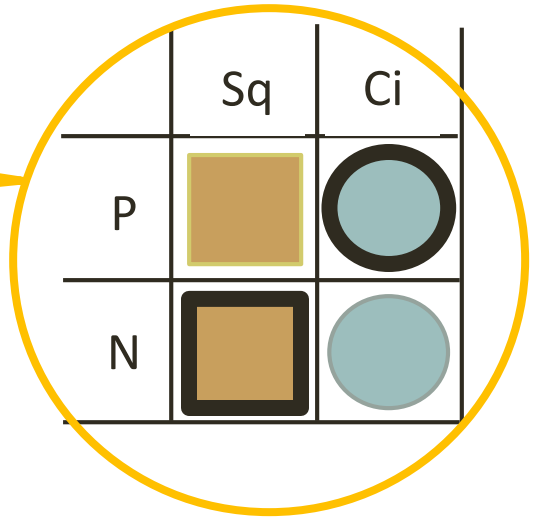
Evaluate Model: Confusion Matrix

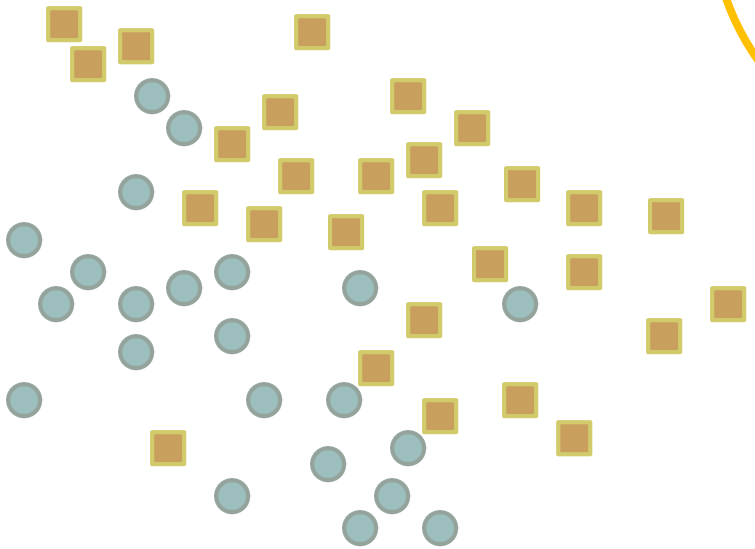


isSquare ~ xLocation + yLocation

Evaluate Model: Confusion Matrix

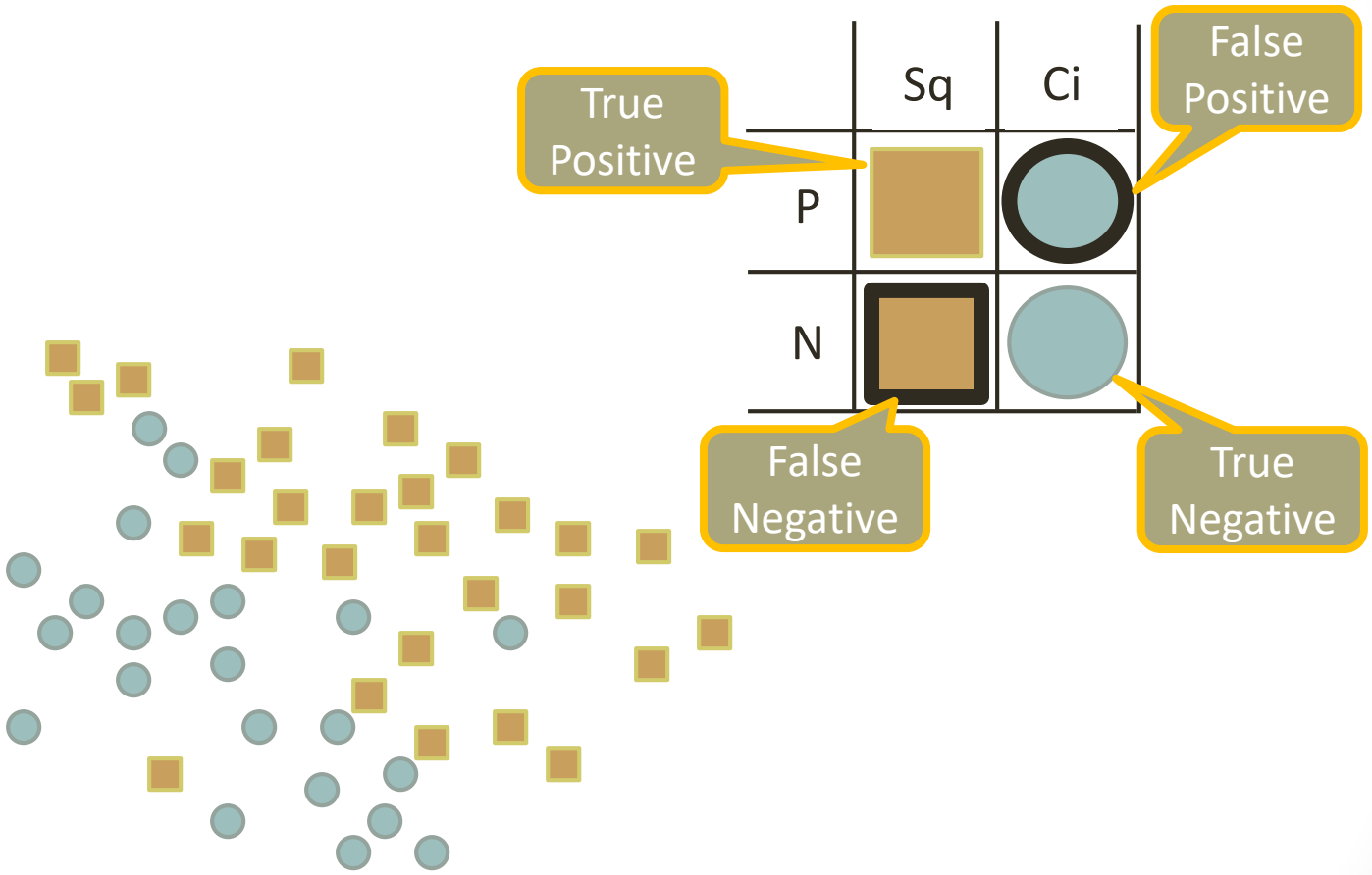
Confusion Matrix (Classification Matrix):
Vertical are actual classes
Horizontal are predicted classes





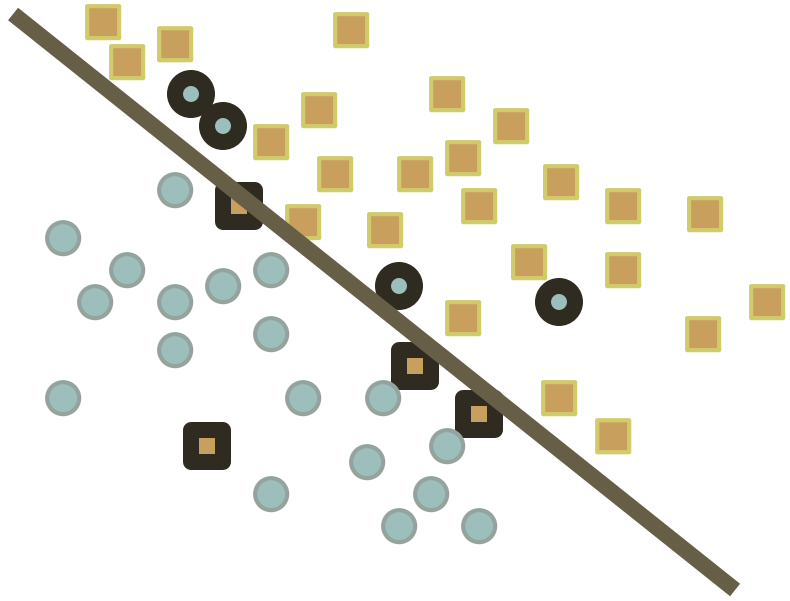
isSquare ~ xLocation + yLocation

Evaluate Model: Confusion Matrix



isSquare ~ xLocation + yLocation

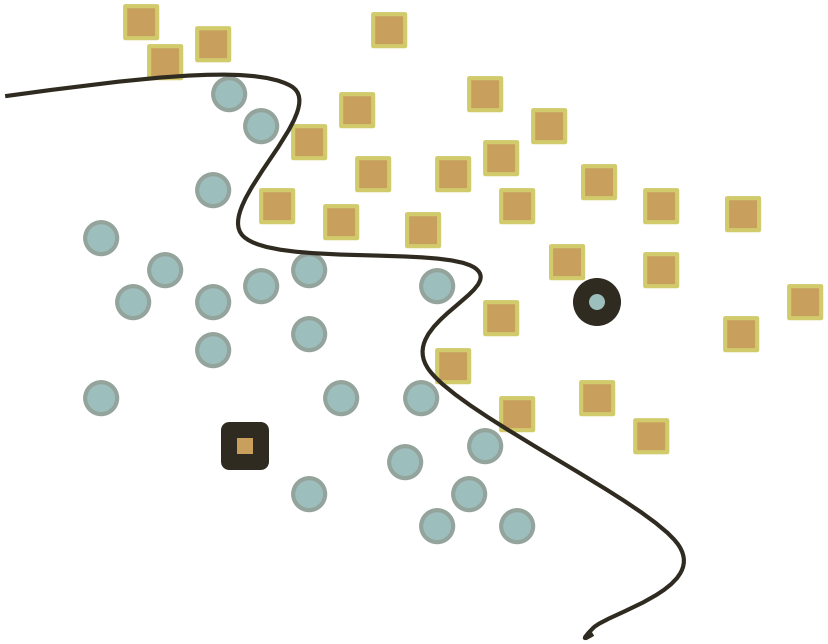
Evaluate Model : Train Model 1



	Sq	Ci
P	36	4
N	4	26

isSquare ~ xLocation + yLocation

Evaluate Model : Train Model 2

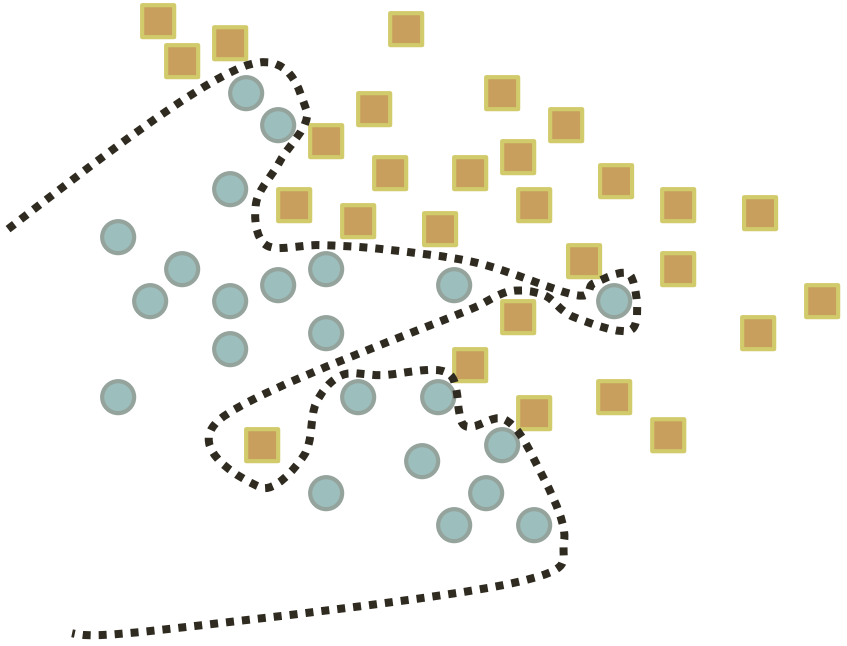


	Sq	Ci
P	39	1
N	1	29

isSquare ~ xLocation + yLocation

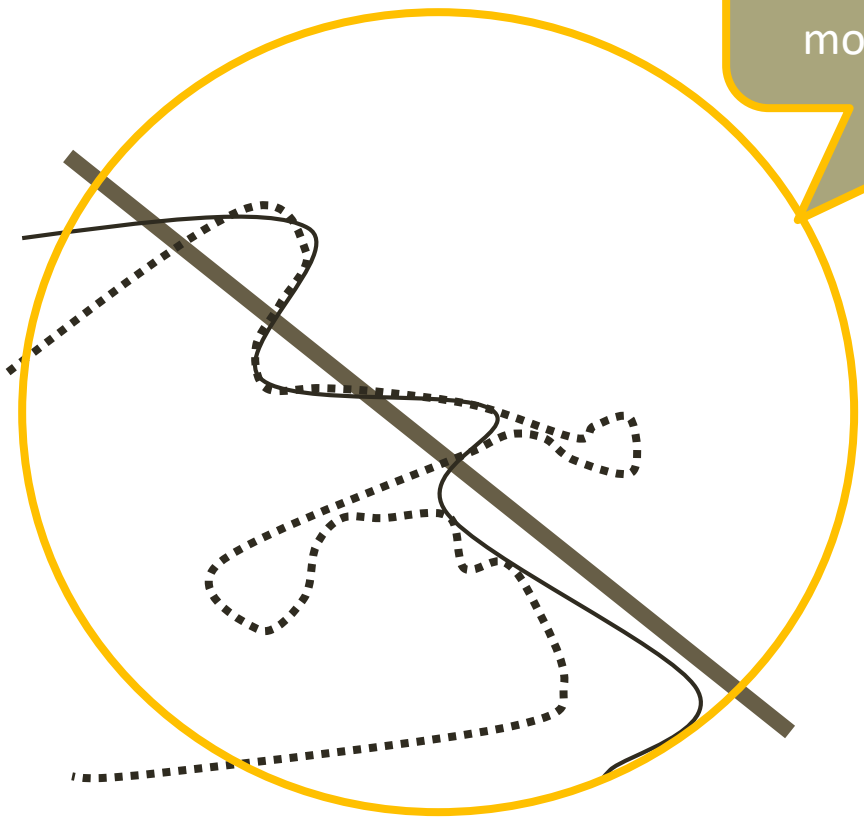
Evaluate Model : Train Model 3

	Sq	Ci
P	40	0
N	0	30



isSquare ~ xLocation + yLocation

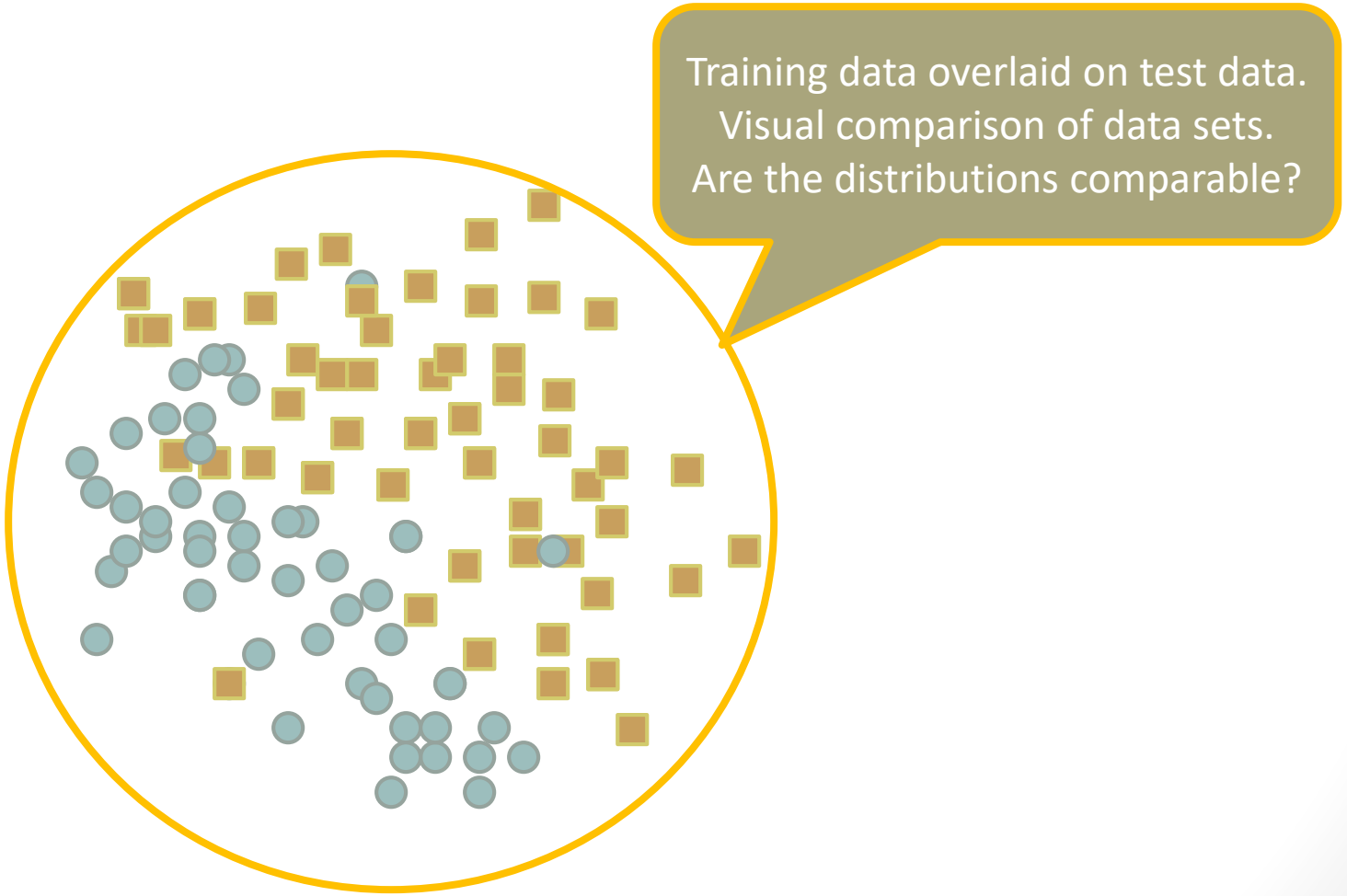
Evaluate Model : 3 Models



These models are based on training data. In these cases, models are called hypotheses.

isSquare ~ xLocation + yLocation

Evaluate Model : All Data

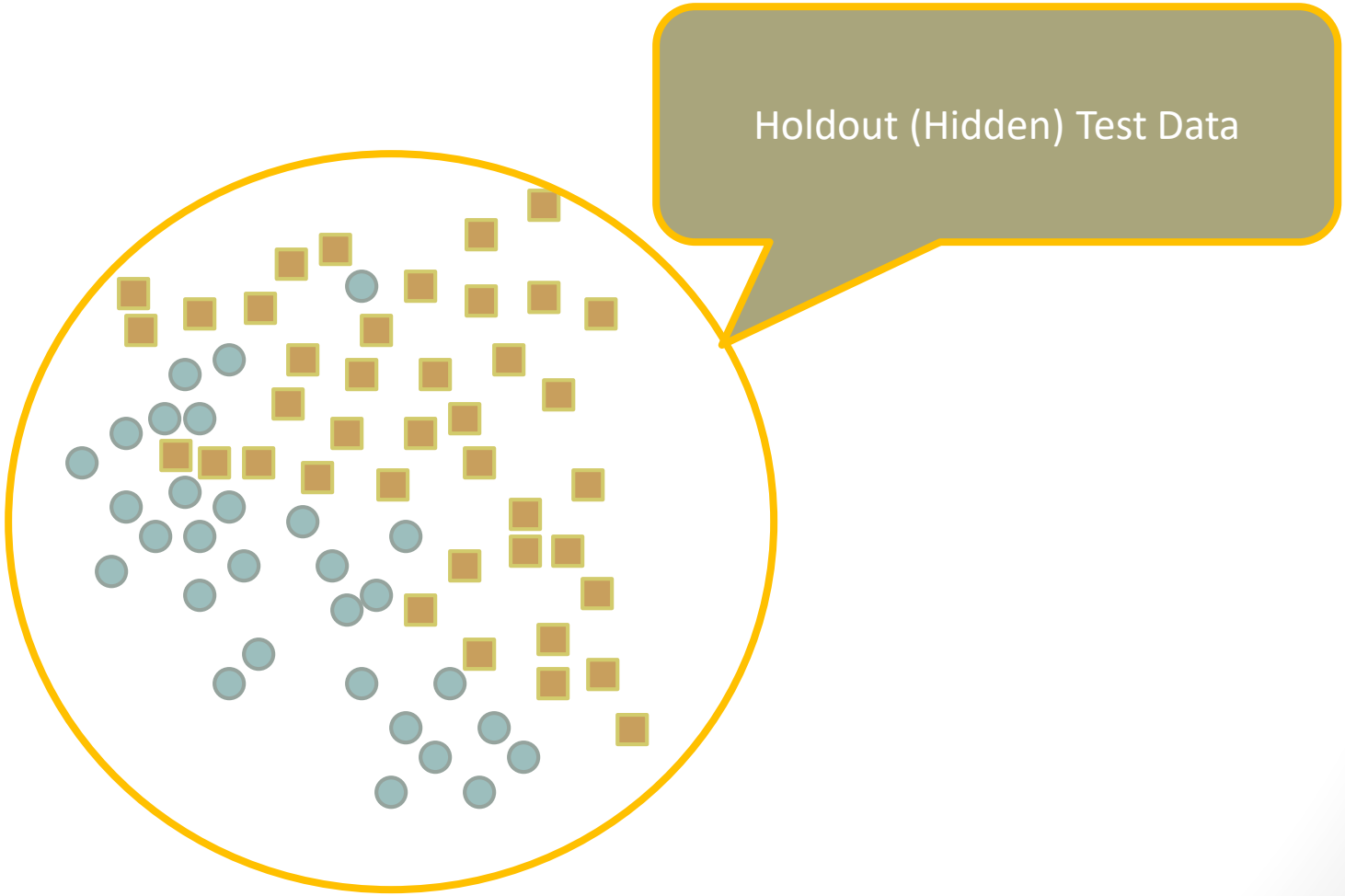


isSquare ~ xLocation + yLocation

Evaluate Model : Training Data

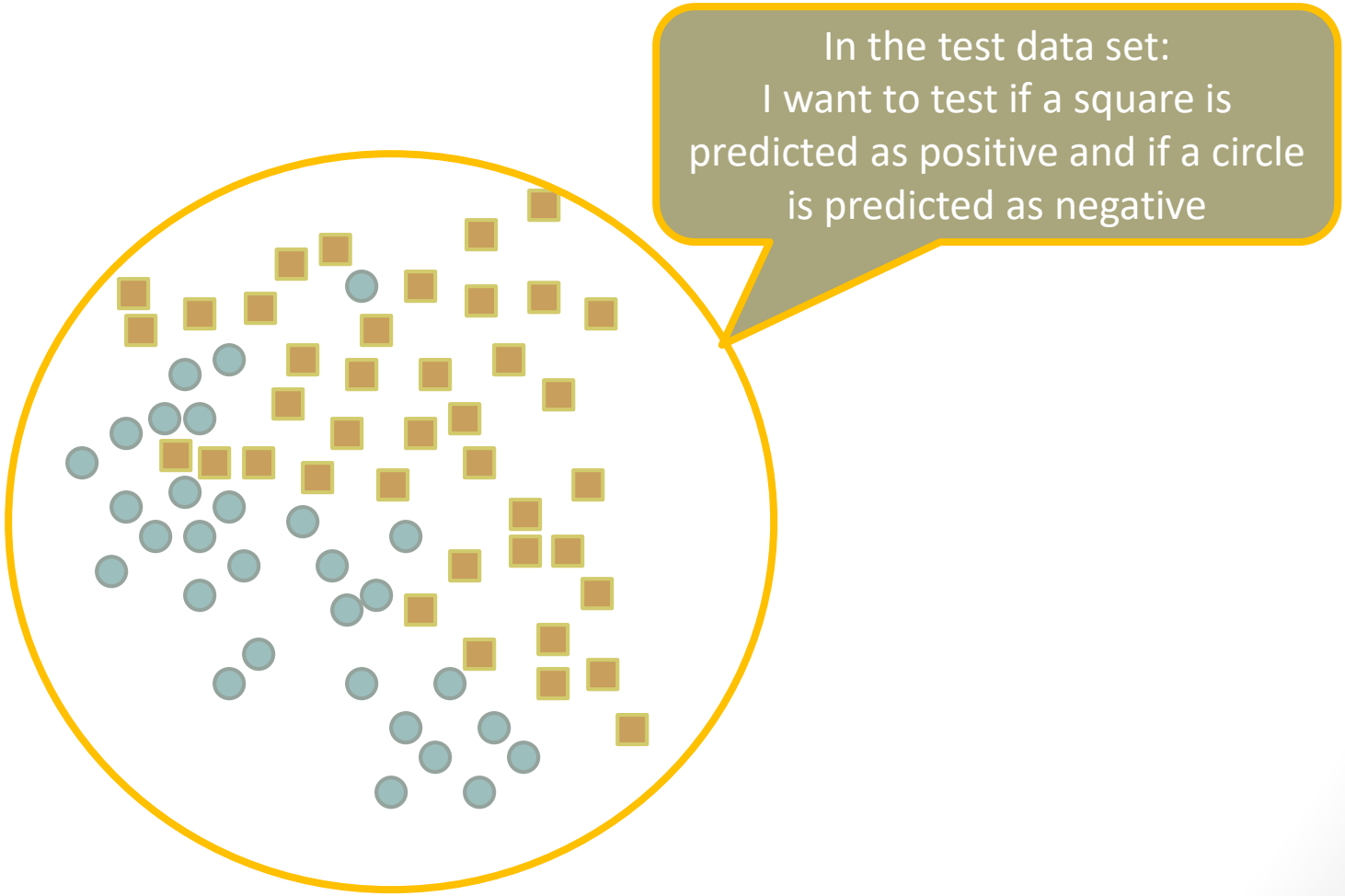
isSquare ~ xLocation + yLocation

Evaluate Model : Test Data



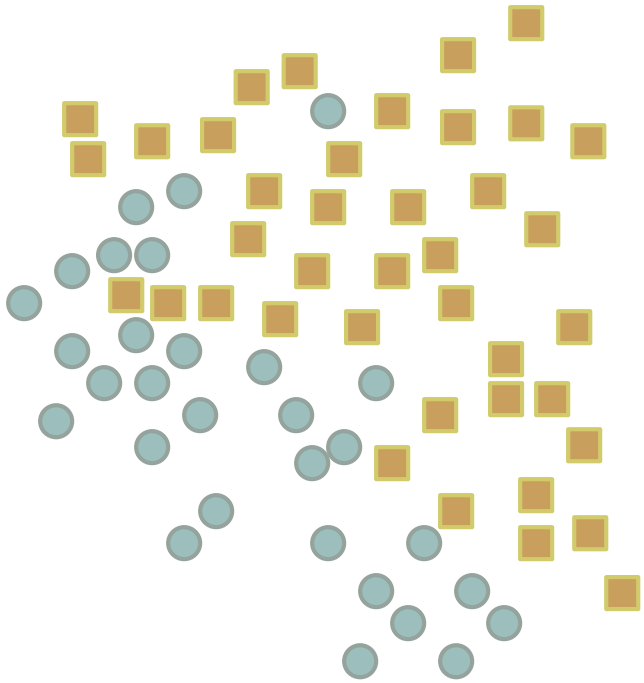
isSquare ~ xLocation + yLocation

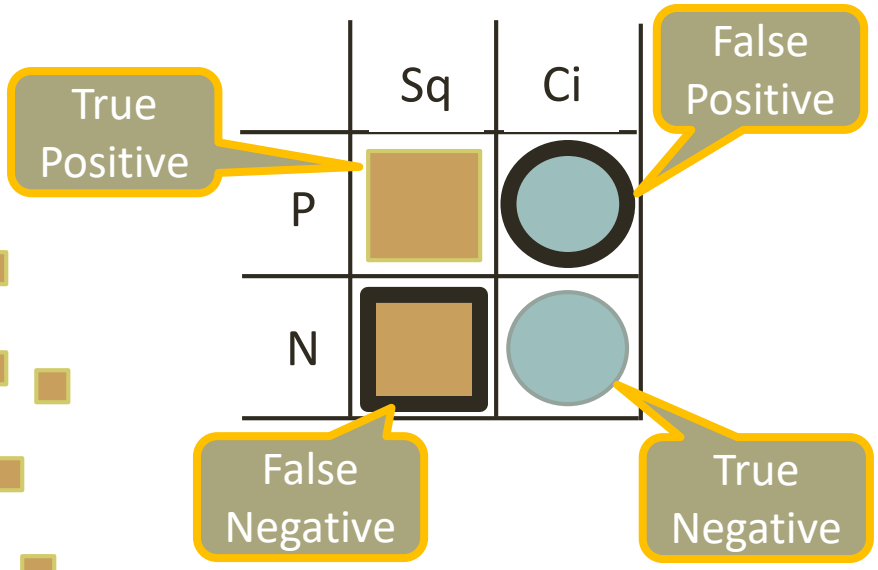
Evaluate Model : Test Data



isSquare ~ xLocation + yLocation

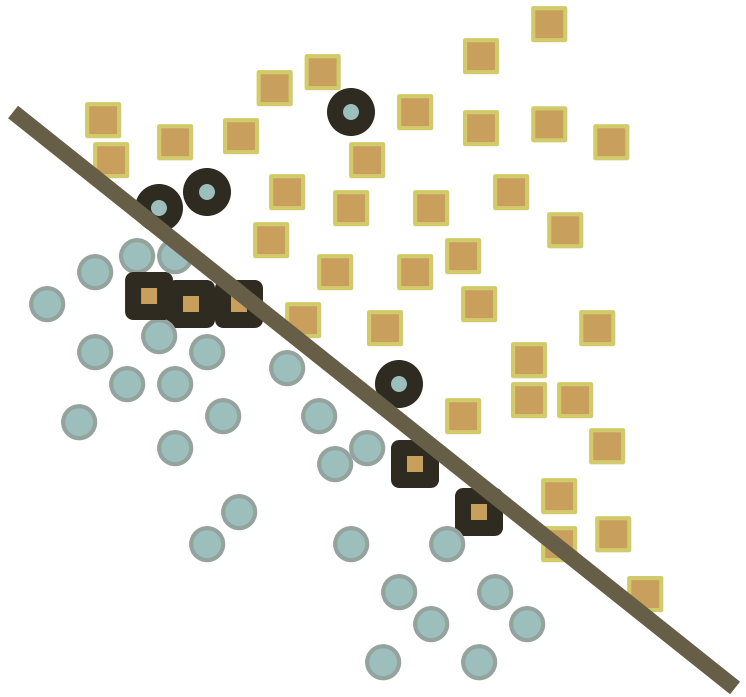
Evaluate Model : Test Data





isSquare ~ xLocation + yLocation

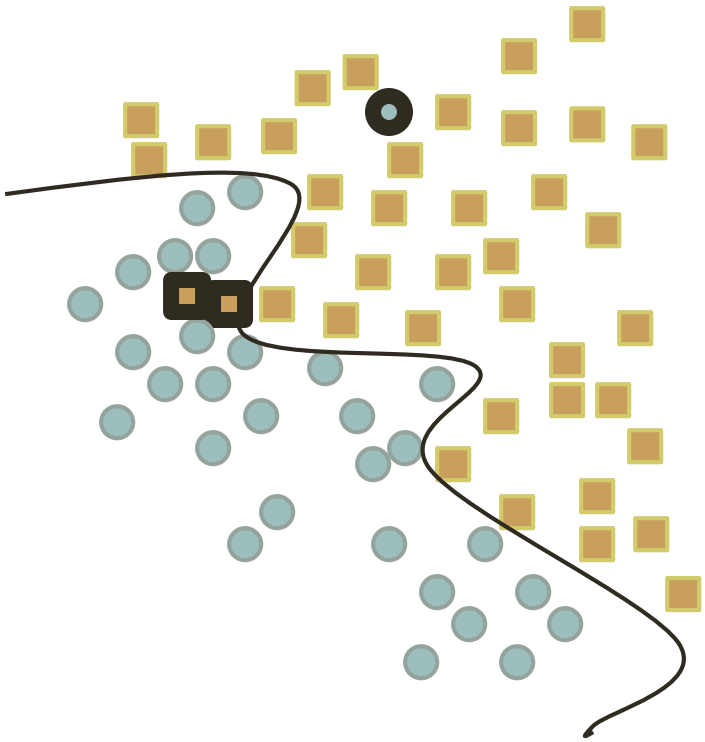
Evaluate Model : Test Model 1



	Sq	Ci
P	35	4
N	5	26

isSquare ~ xLocation + yLocation

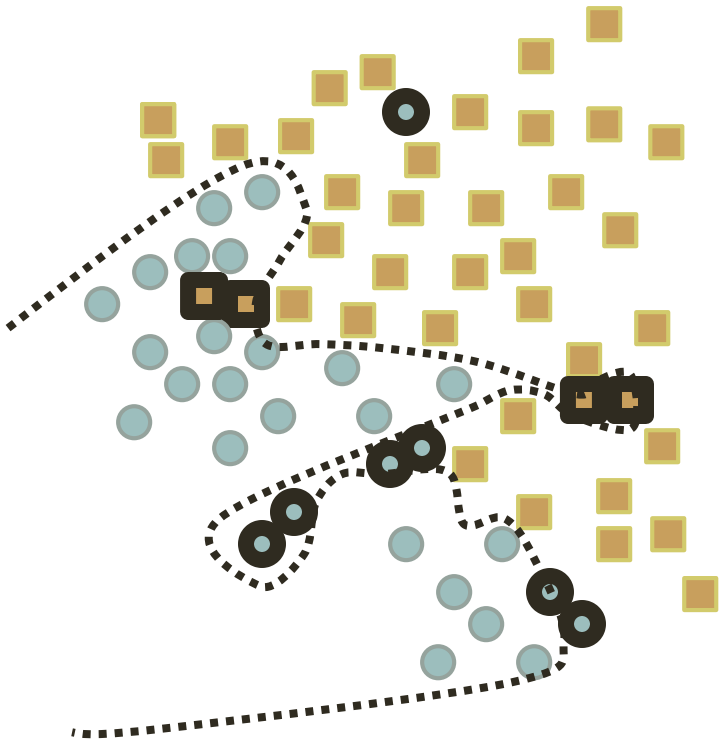
Evaluate Model : Test Model 2



	Sq	Ci
P	38	1
N	2	29

isSquare ~ xLocation + yLocation

Evaluate Model : Test Model 3



	Sq	Ci
P	36	7
N	4	23

isSquare ~ xLocation + yLocation

Over-fitting and Confusion Matrix

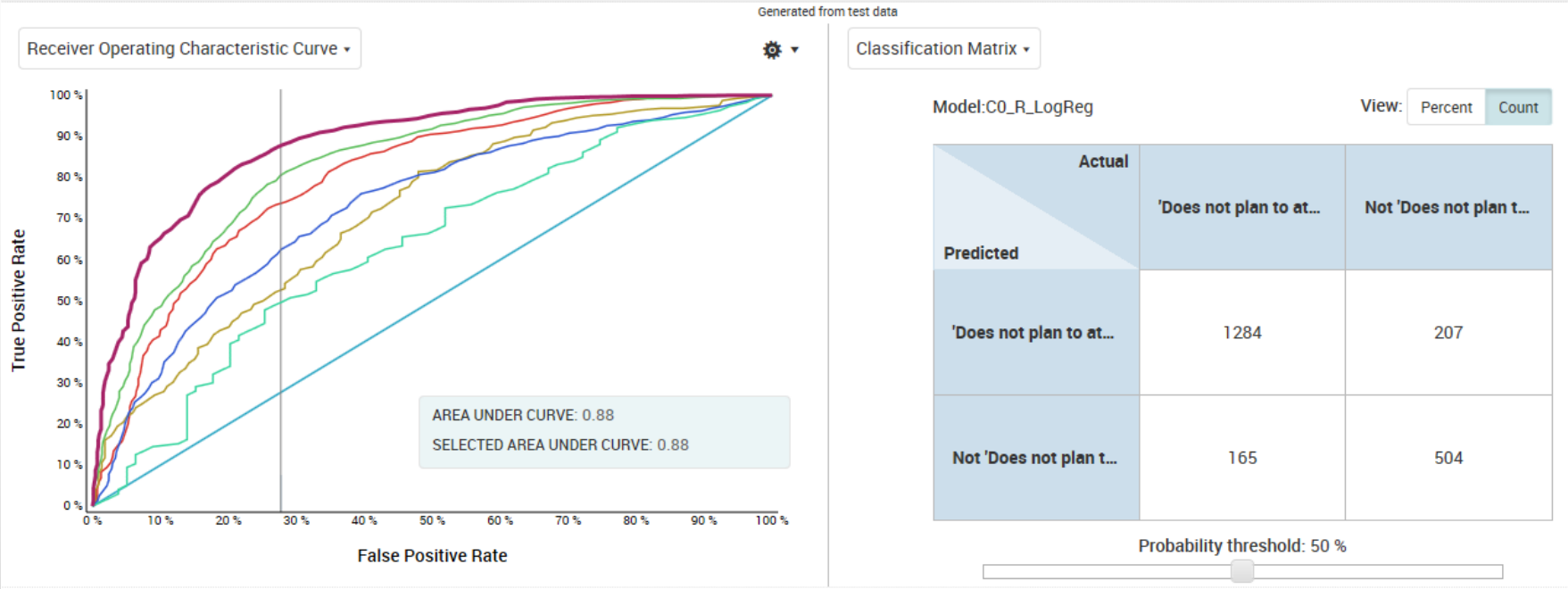
Lesson 09 Quiz 0a Confusion Matrix

- Quiz Confusion Matrix
  - Test and Accuracy Measures

ROC Chart Intro

ROC Chart Intro (1)

- Confusion Matrix and ROC Chart

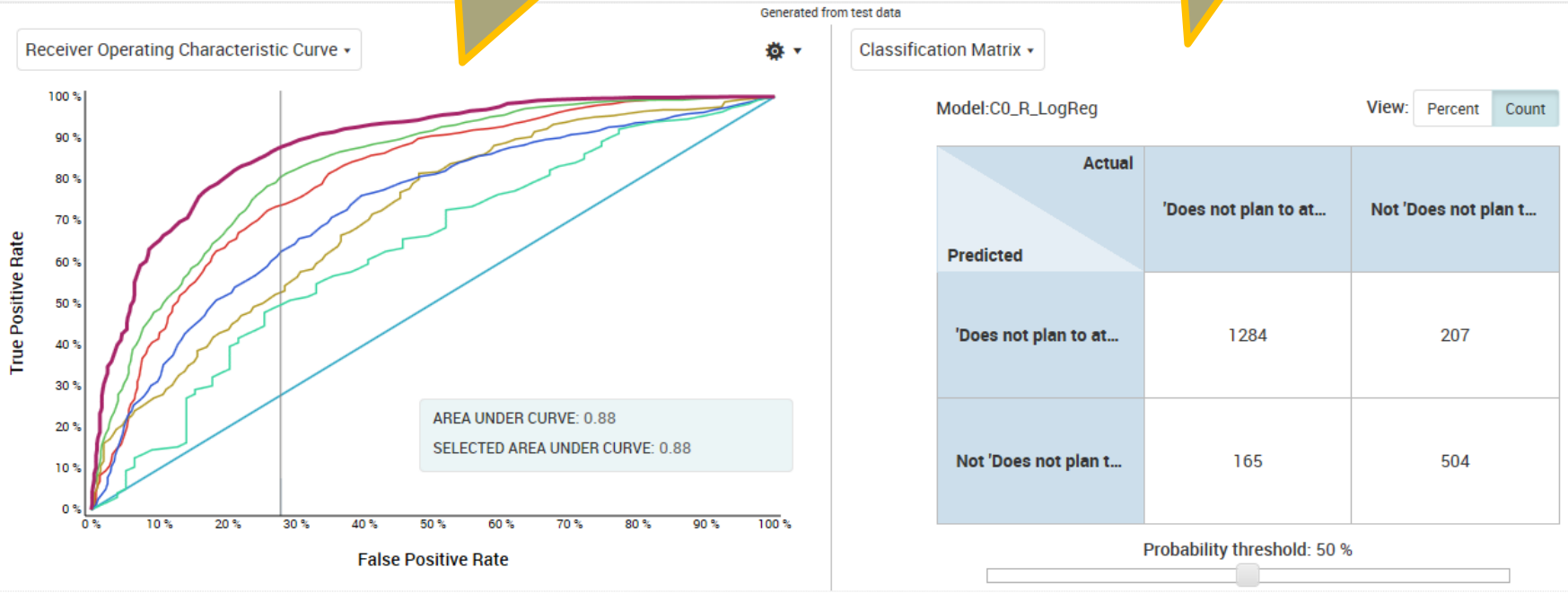


ROC Chart Intro (2)

- Confusion Matrix and ROC Chart

Comparison of 6 ROC curves
Each curve is from a different model

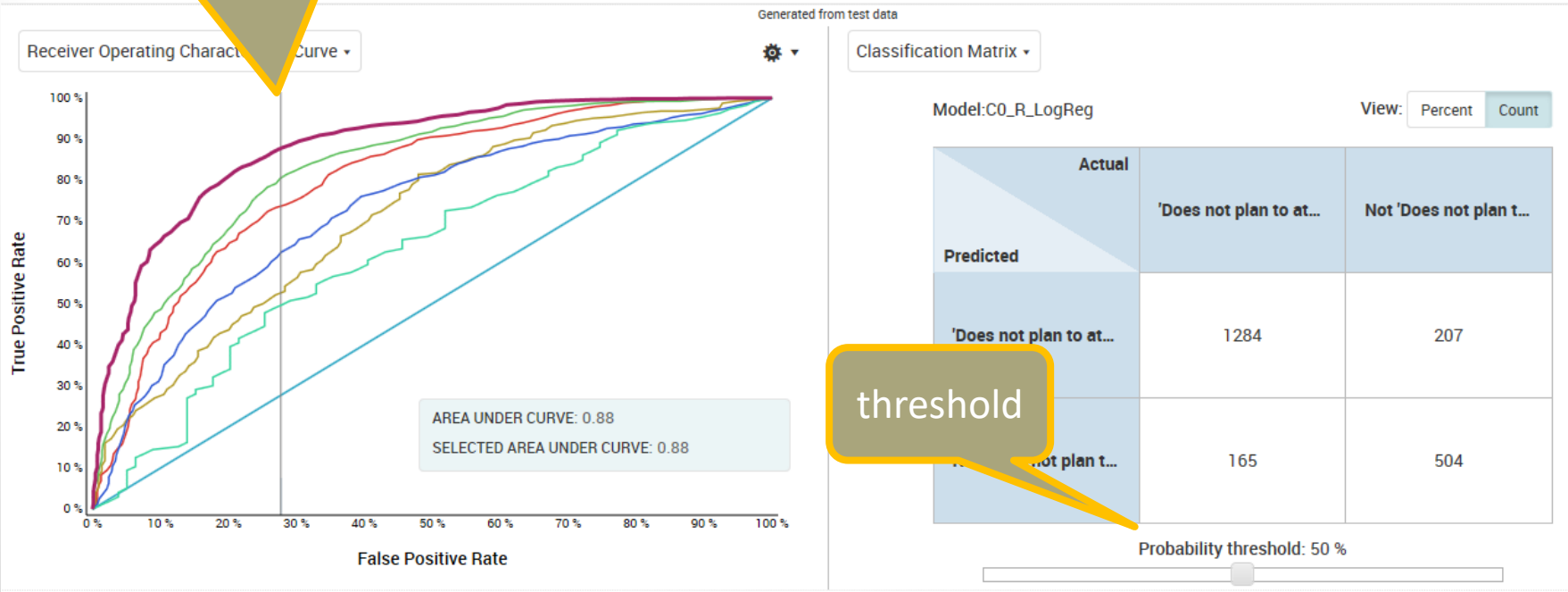
The confusion matrix for one model at one threshold



ROC Chart Intro (3)

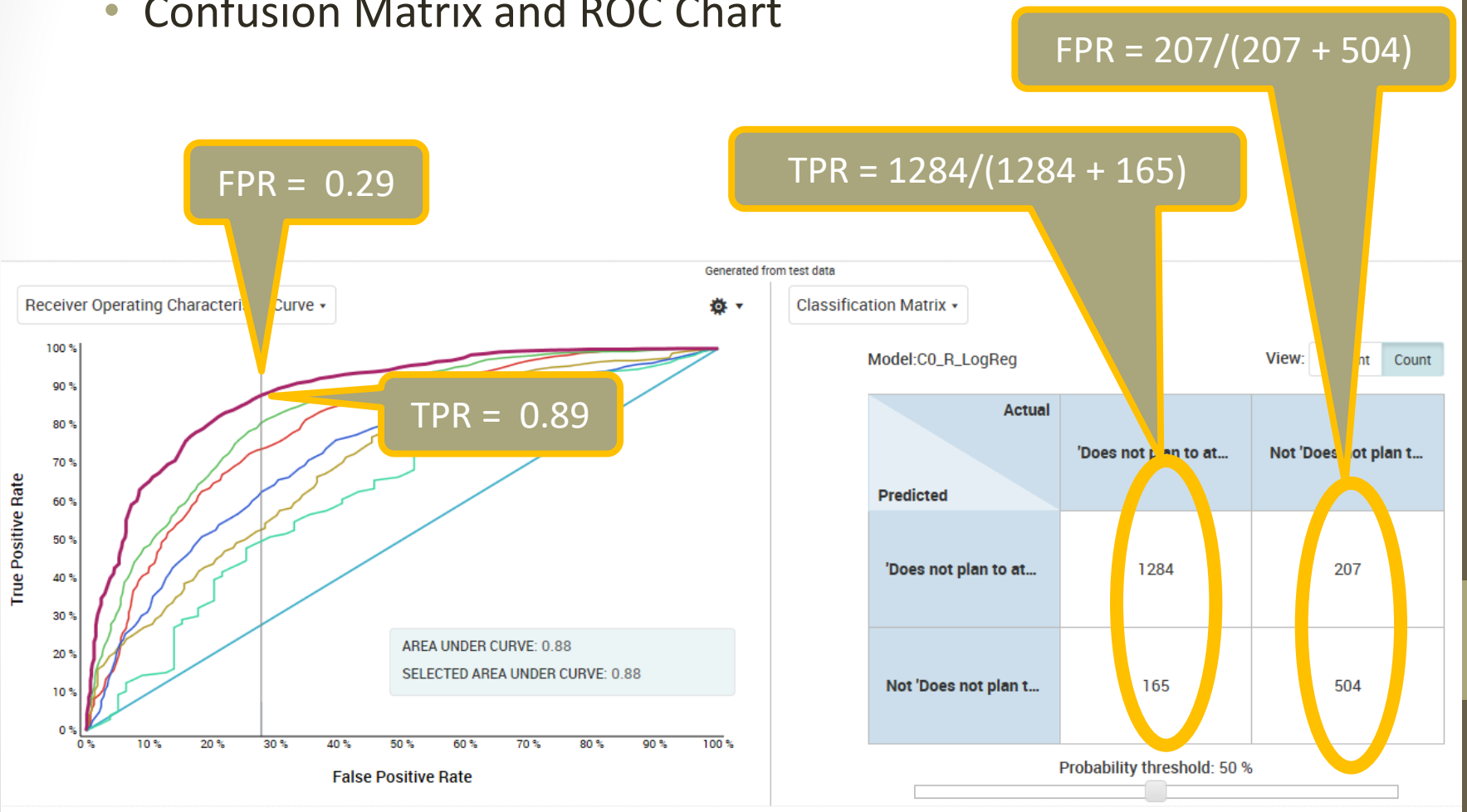
- Confusion Matrix and ROC Chart

This FPR (0.28) corresponds to the threshold (0.5) for the confusion matrix for the best model



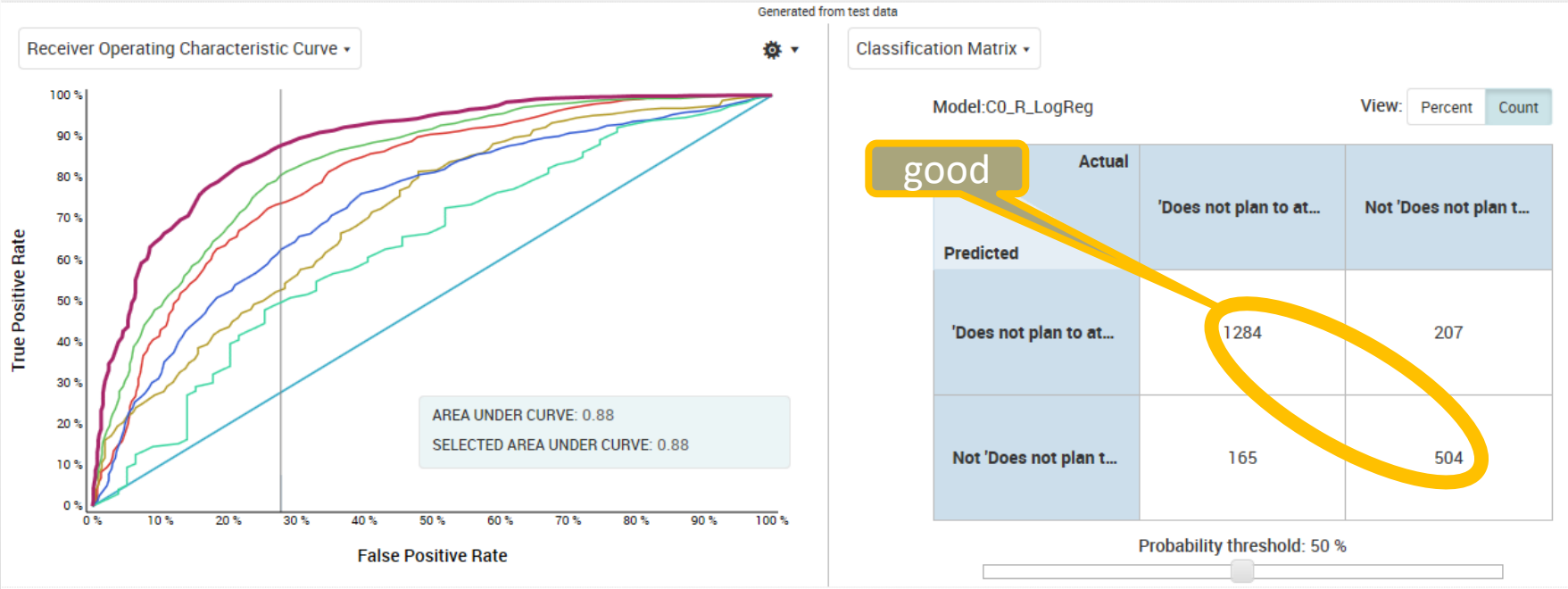
ROC Chart Intro (4)

- Confusion Matrix and ROC Chart



ROC Chart Intro (5)

- Confusion Matrix and ROC Chart



ROC Chart Intro (6)

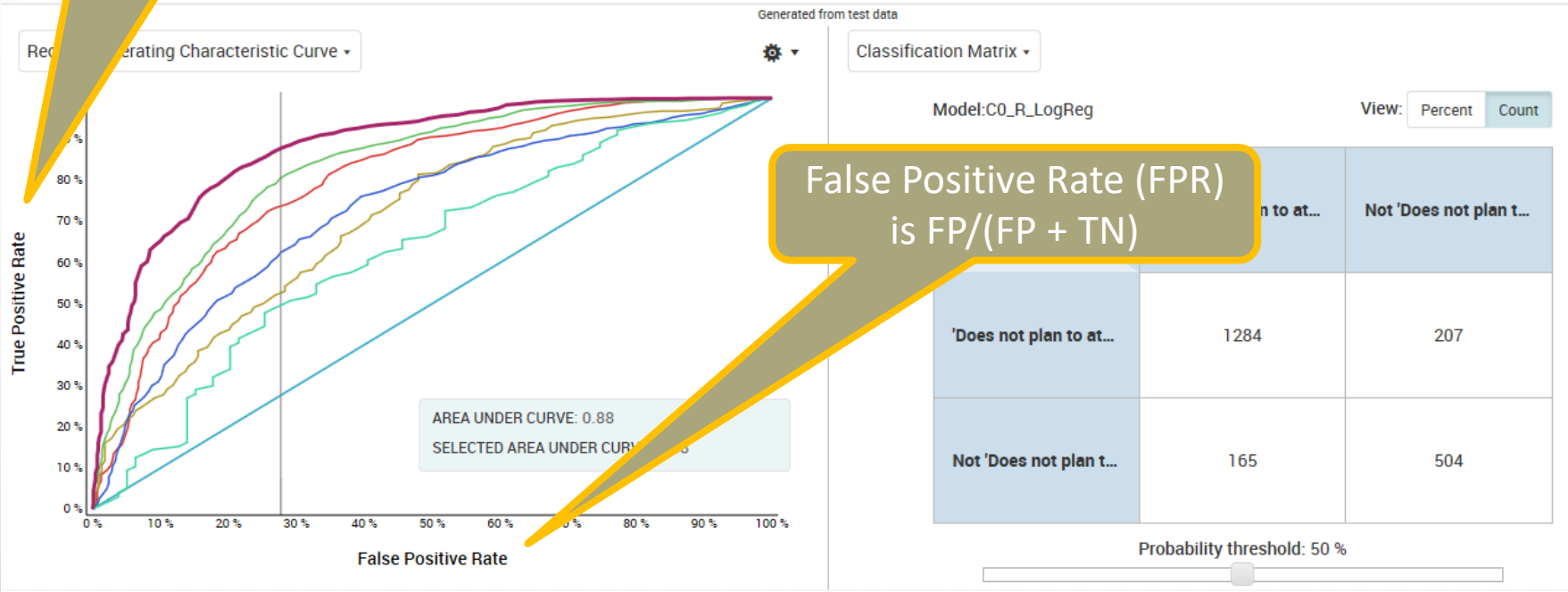
- Confusion Matrix and ROC Chart

ROC Chart Intro (7)

- Confusion Matrix and ROC Chart

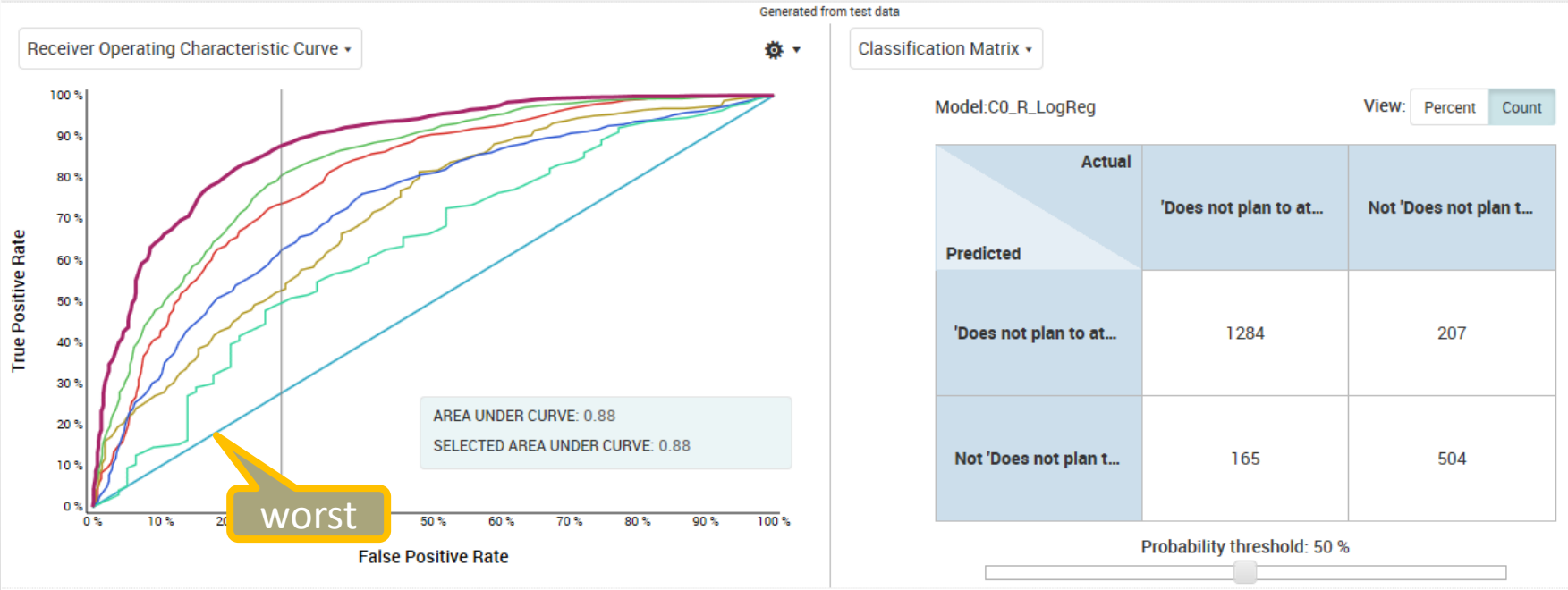
True Positive Rate (TPR) is TP/(TP + FN)

False Positive Rate (FPR) is FP/(FP + TN)



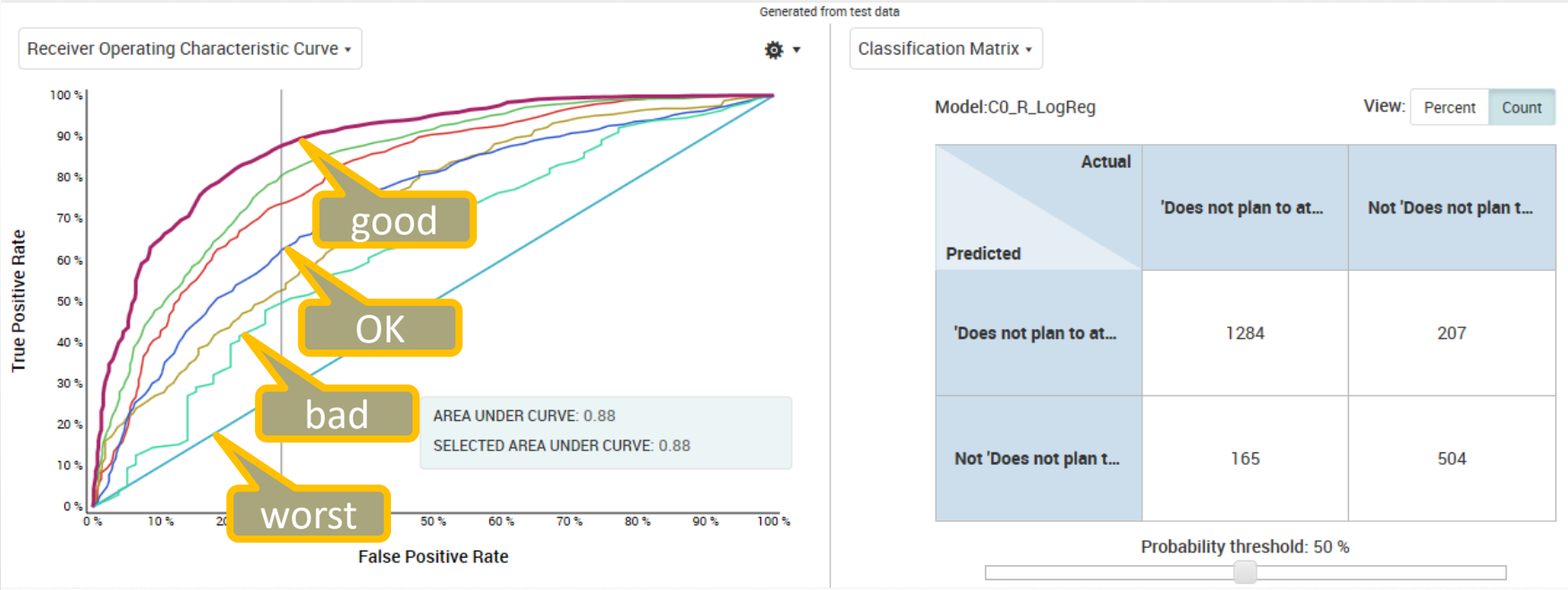
ROC Chart Intro (8)

- Confusion Matrix and ROC Chart



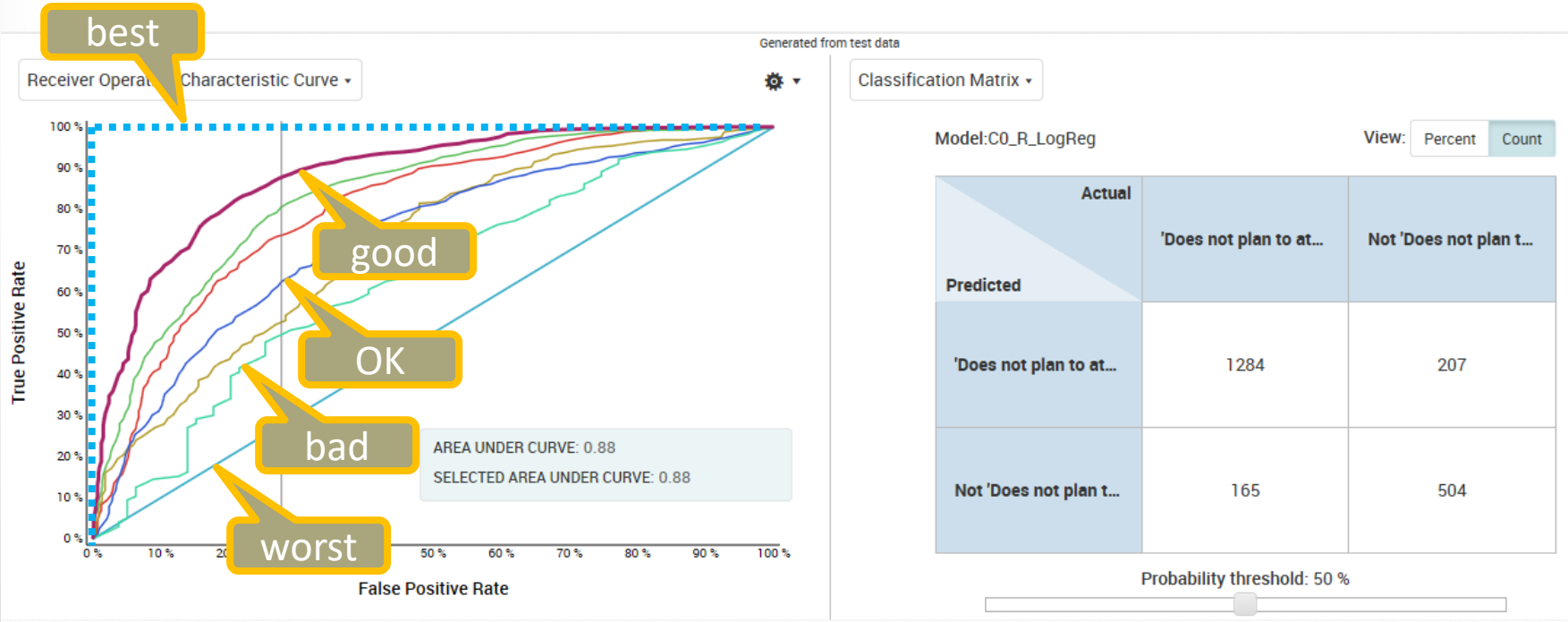
ROC Chart Intro (9)

- Confusion Matrix and ROC Chart



ROC Chart Intro (10)

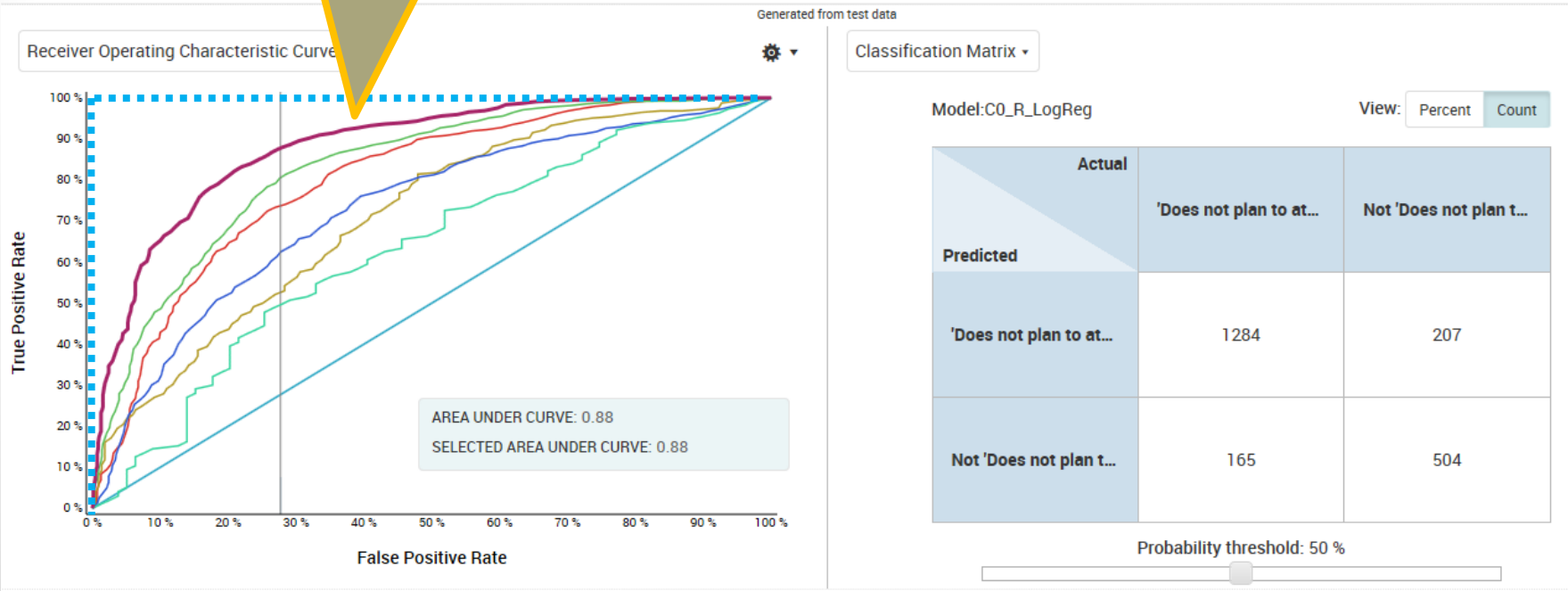
- Confusion Matrix and ROC Chart



ROC Chart Intro (11)

- Confusion Matrix and ROC Chart

ROC charts are non-decreasing functions



ROC Chart Intro

Lesson 09 Quiz 0b ROC Intro

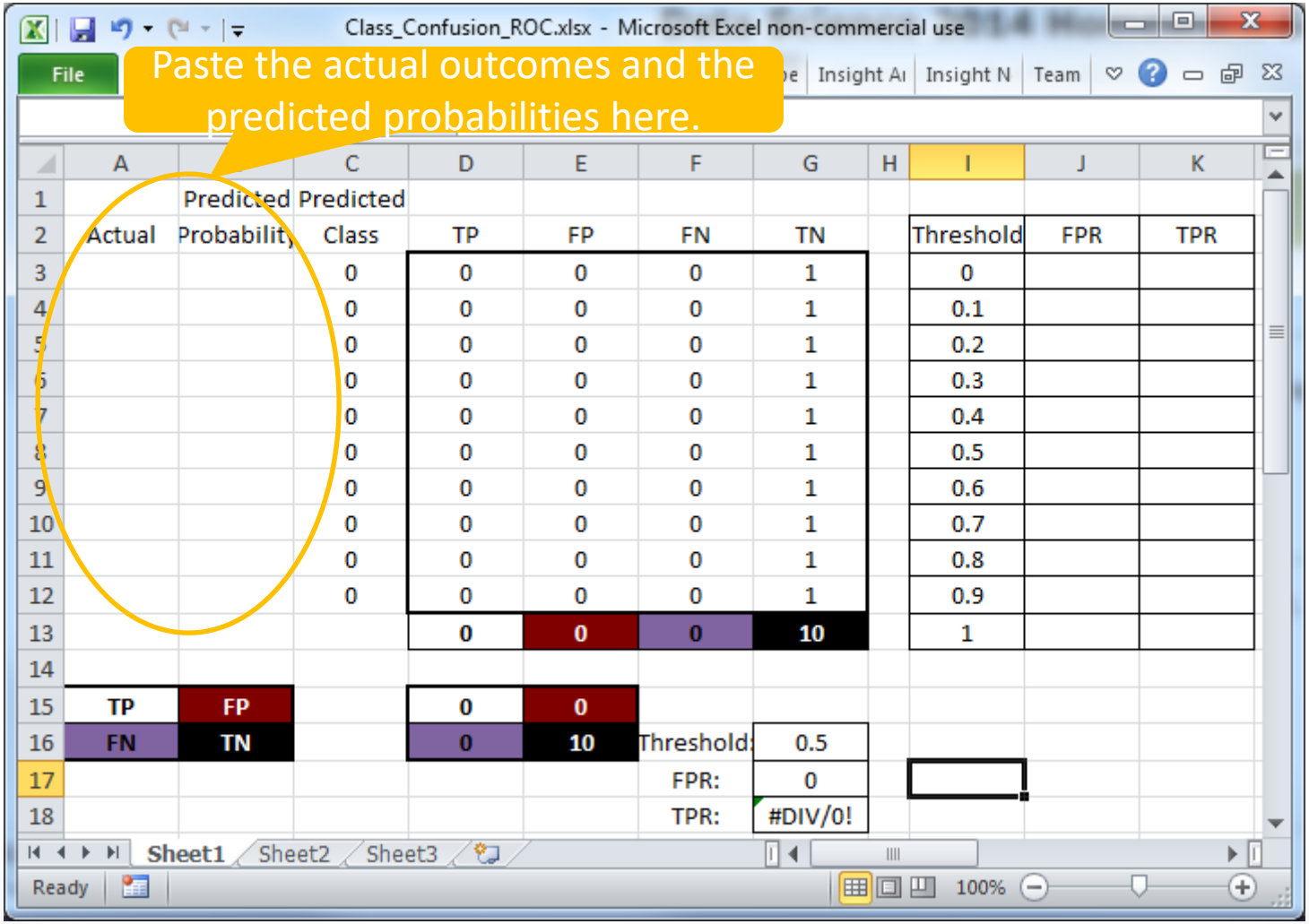
- Quiz ROC Intro

How to make an ROC

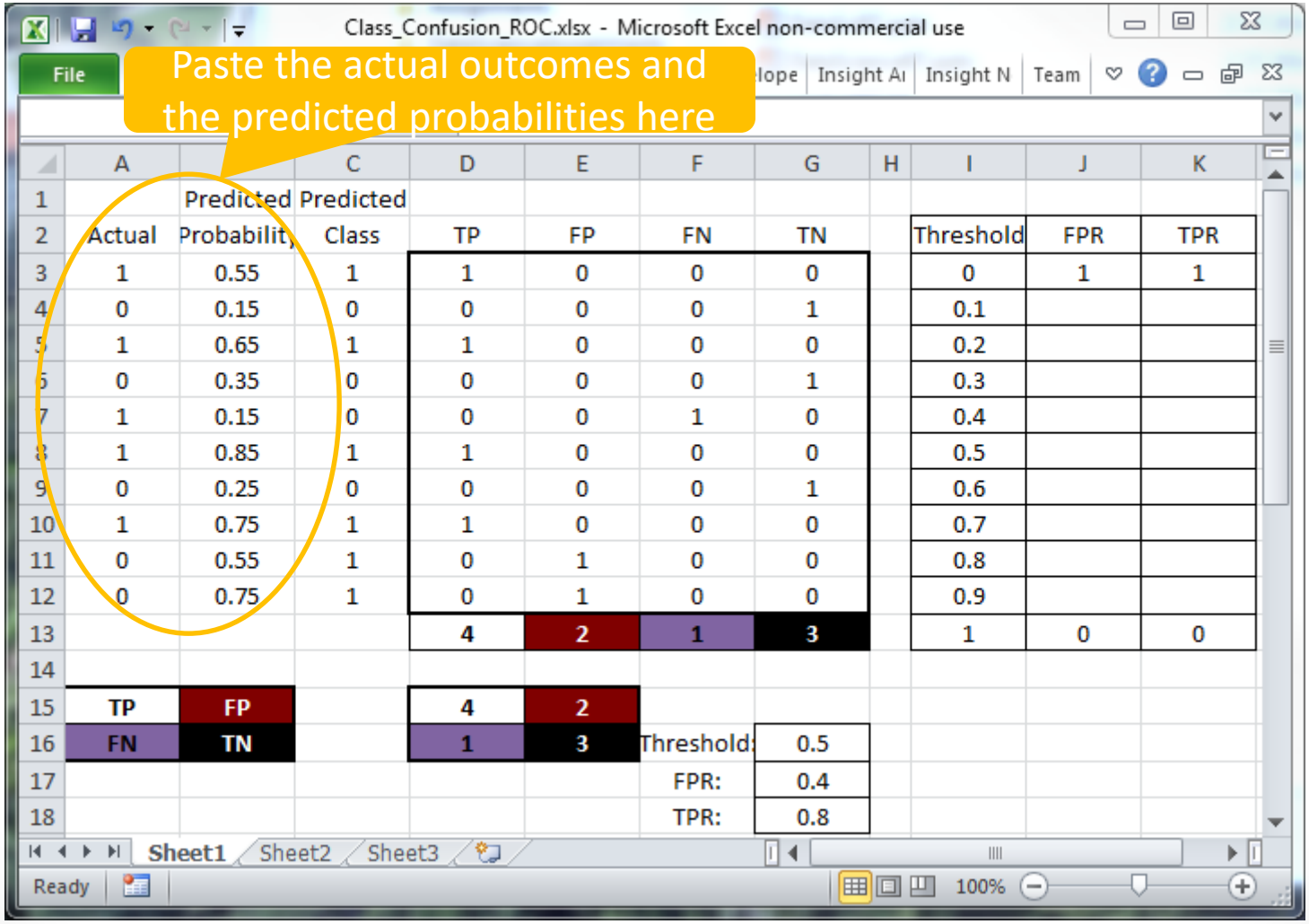
How to make an ROC (0)

- From Probabilities to ROC:
- Probabilities -> Threshold -> Predictions -> Confusion Matrix -> ROC
- Get Excel workbook: HowToMakeAnROC.xls
- Note that at the bottom of the worksheet are the actual outcomes and the predicted probabilities.

How to make an ROC (1)

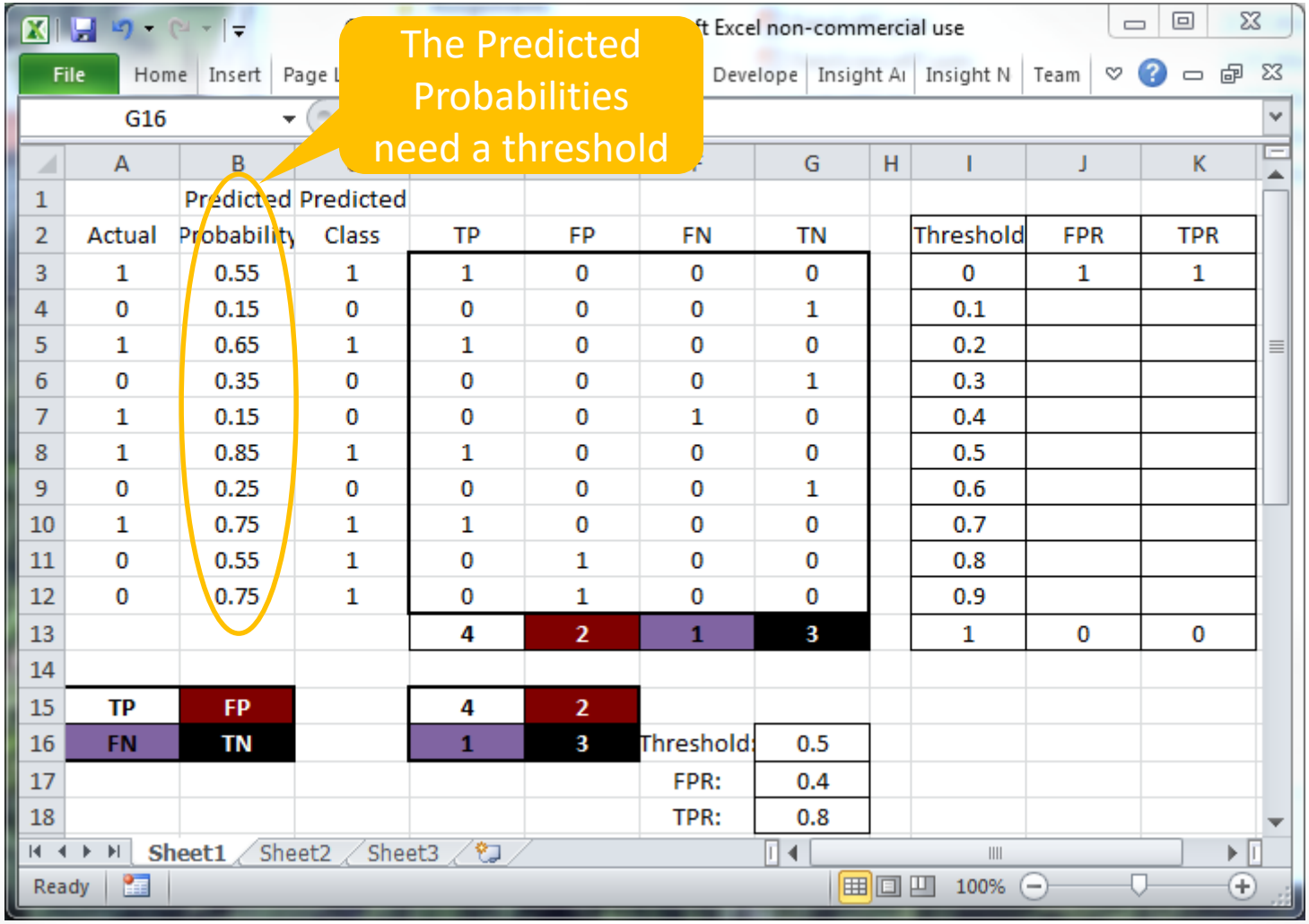


How to make an ROC (2)



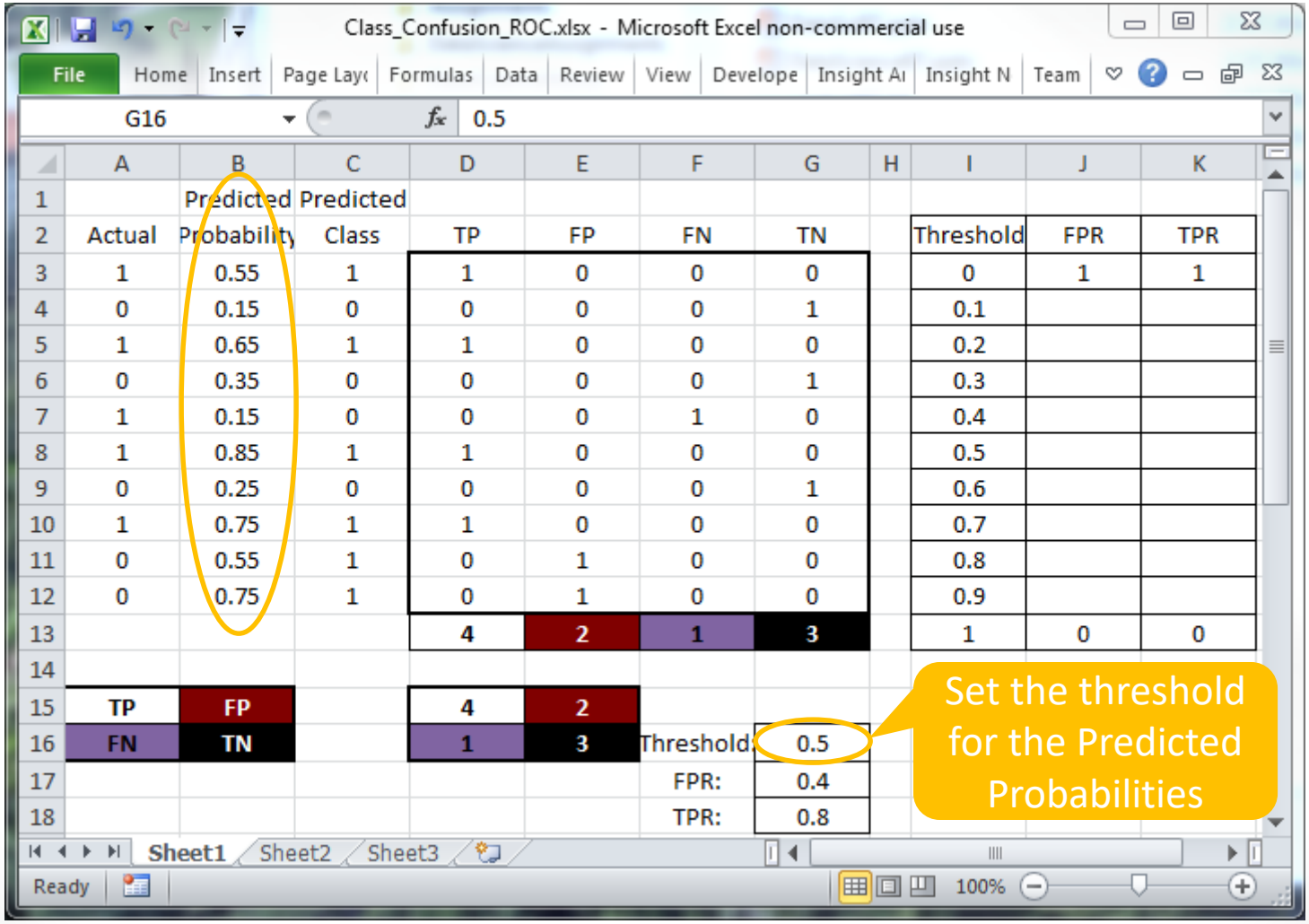
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (3)



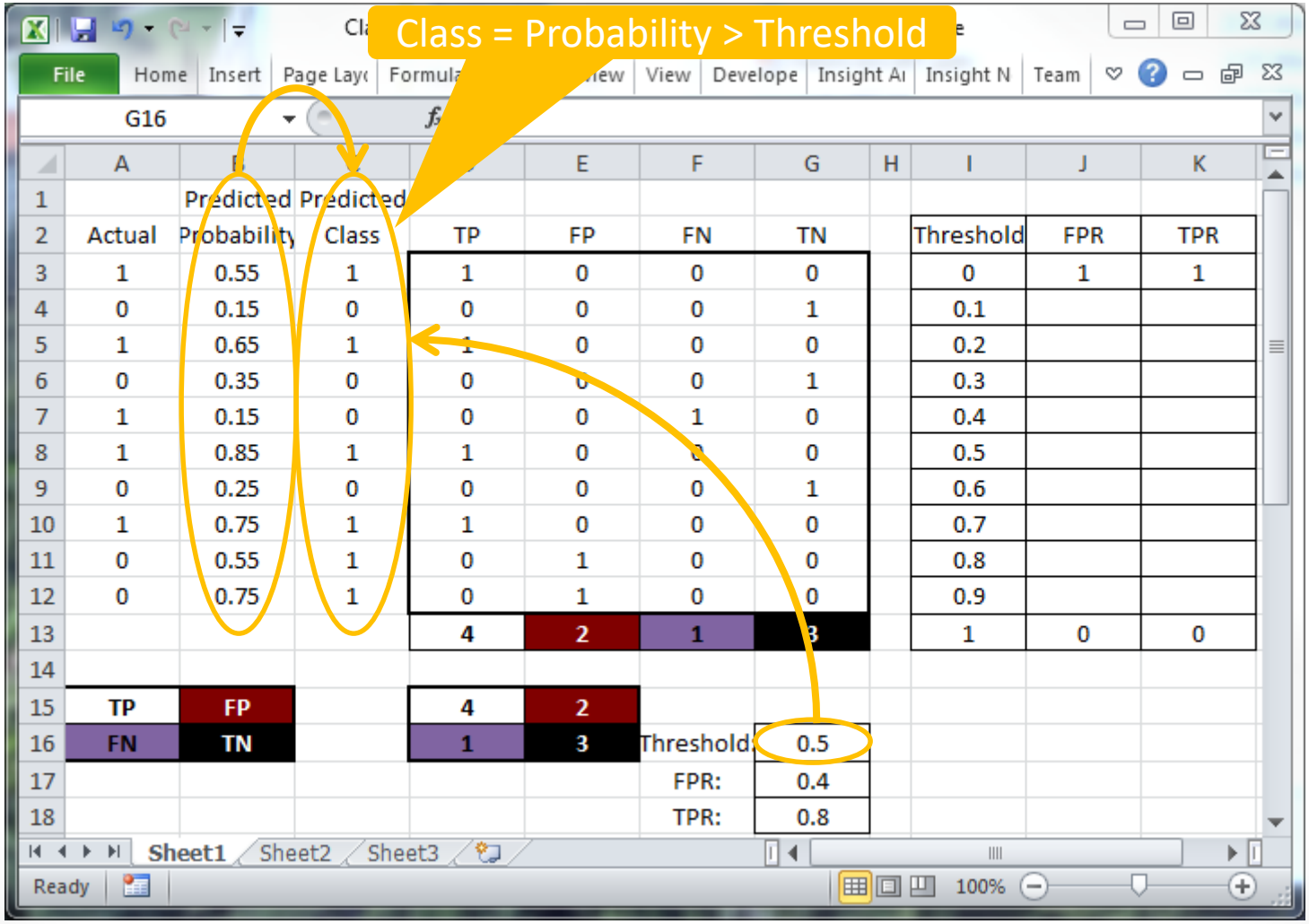
	A	B	C	TP	FP	FN	TN		Threshold	FPR	TPR
1		Predicted	Predicted								
2	Actual	Probability	Class								
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (4)



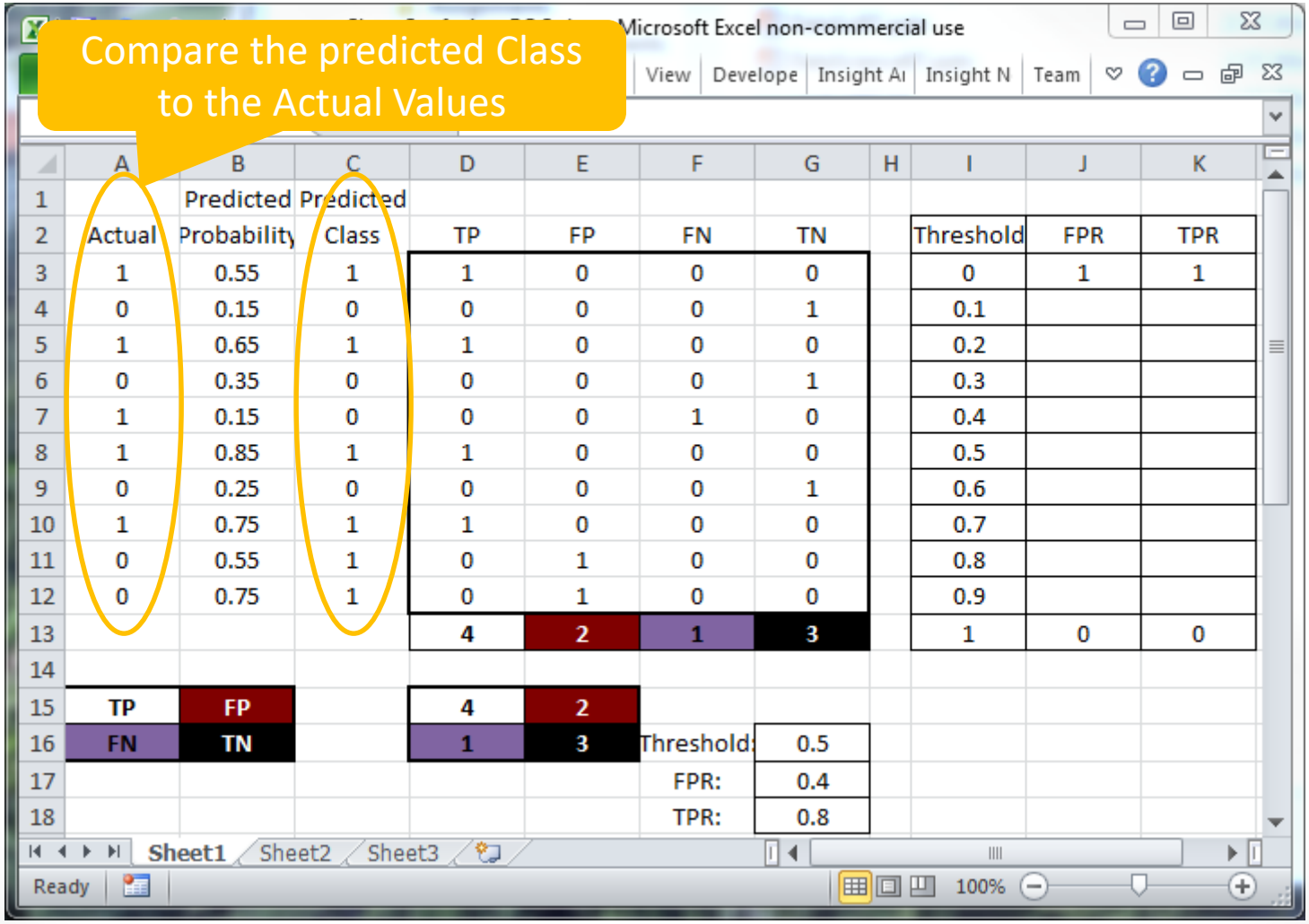
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (5)



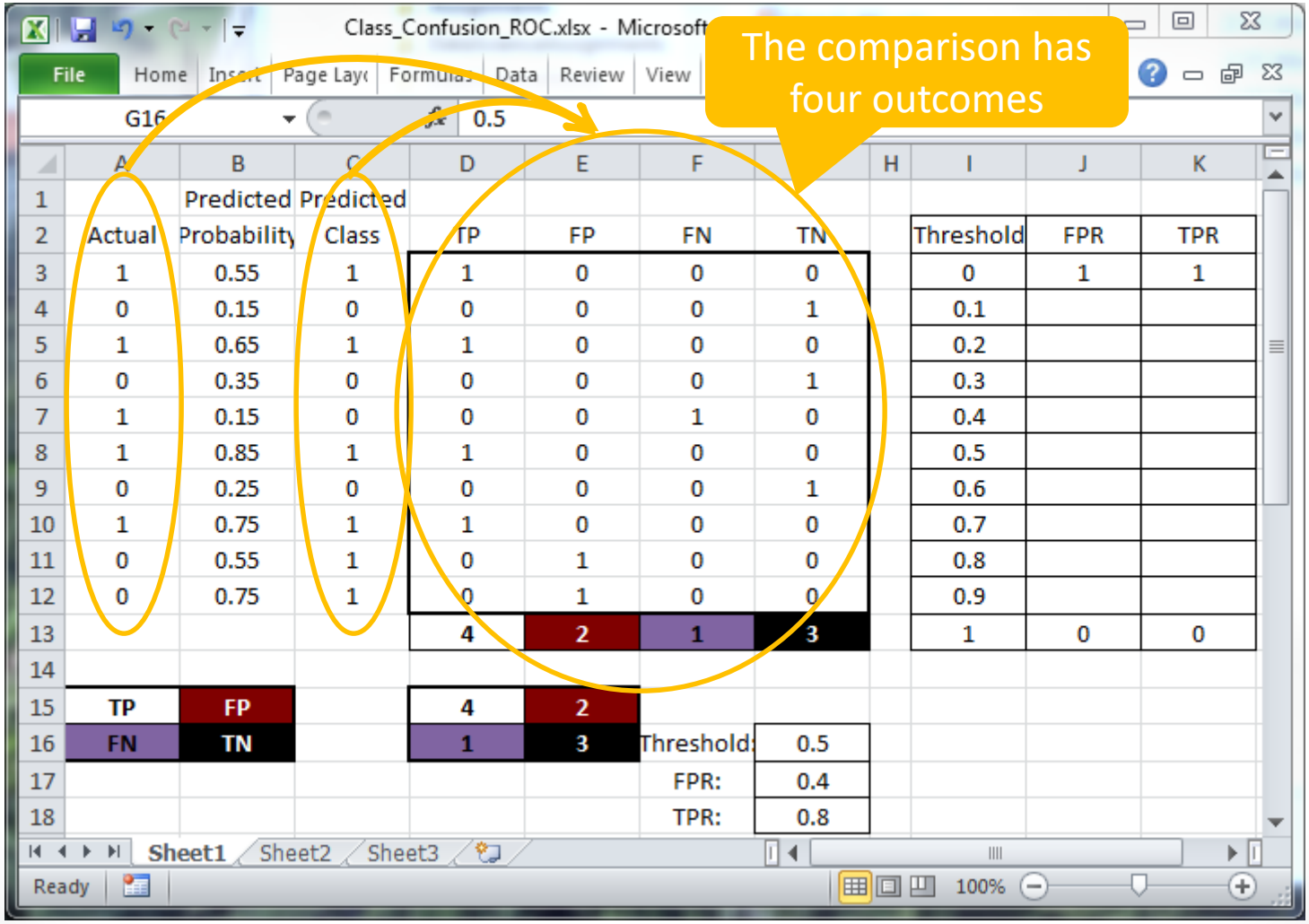
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (6)



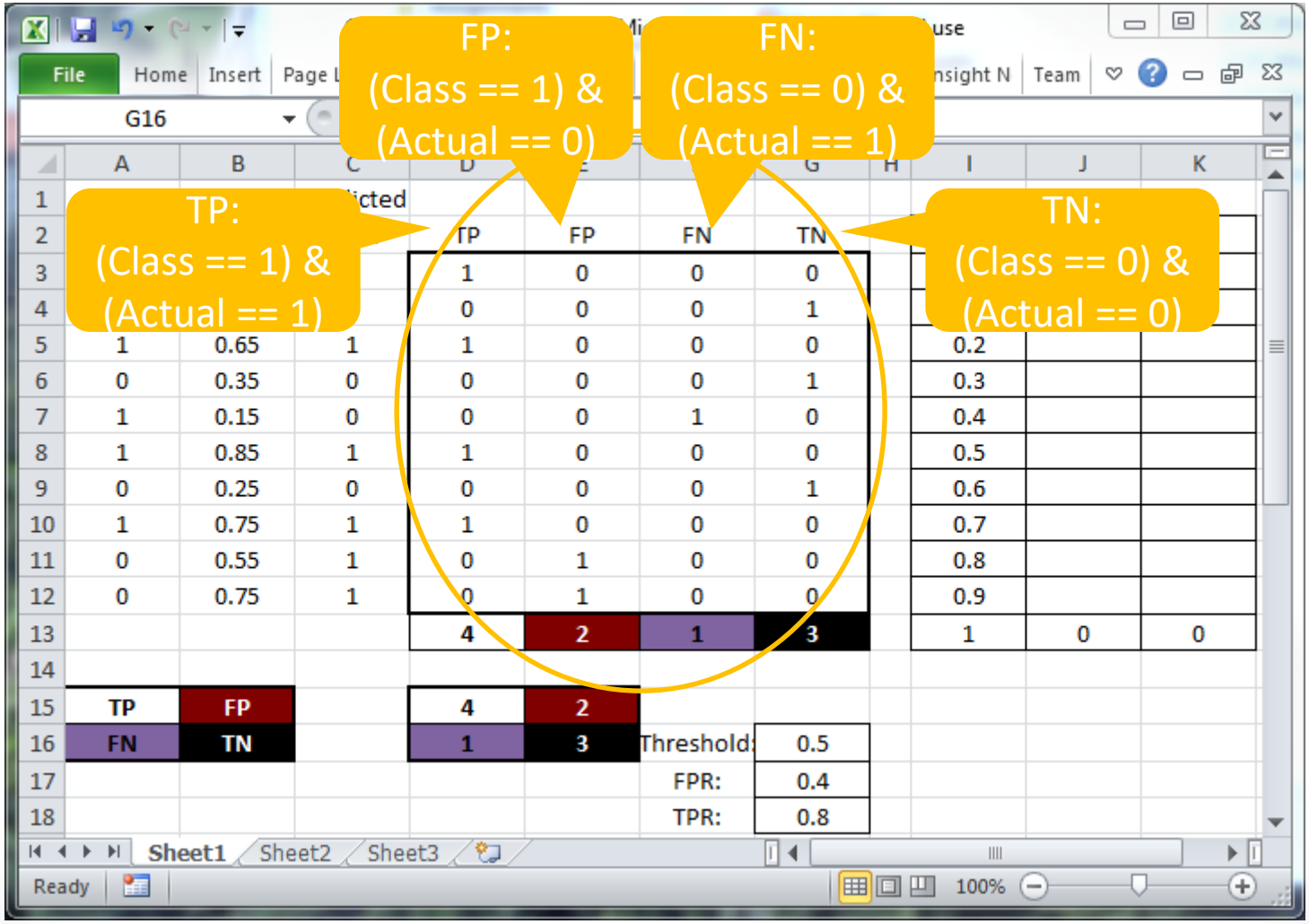
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (7)

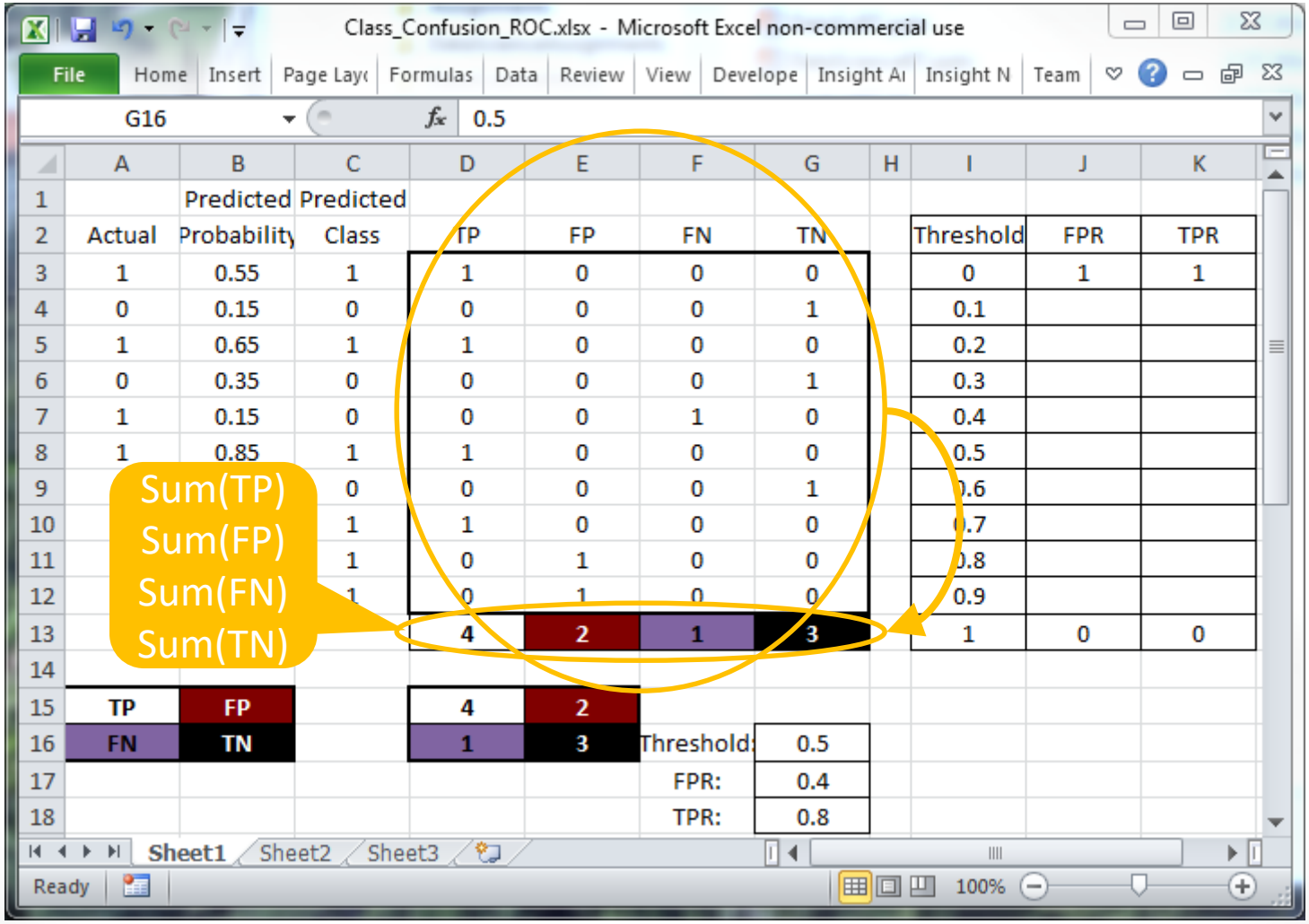


	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (8)

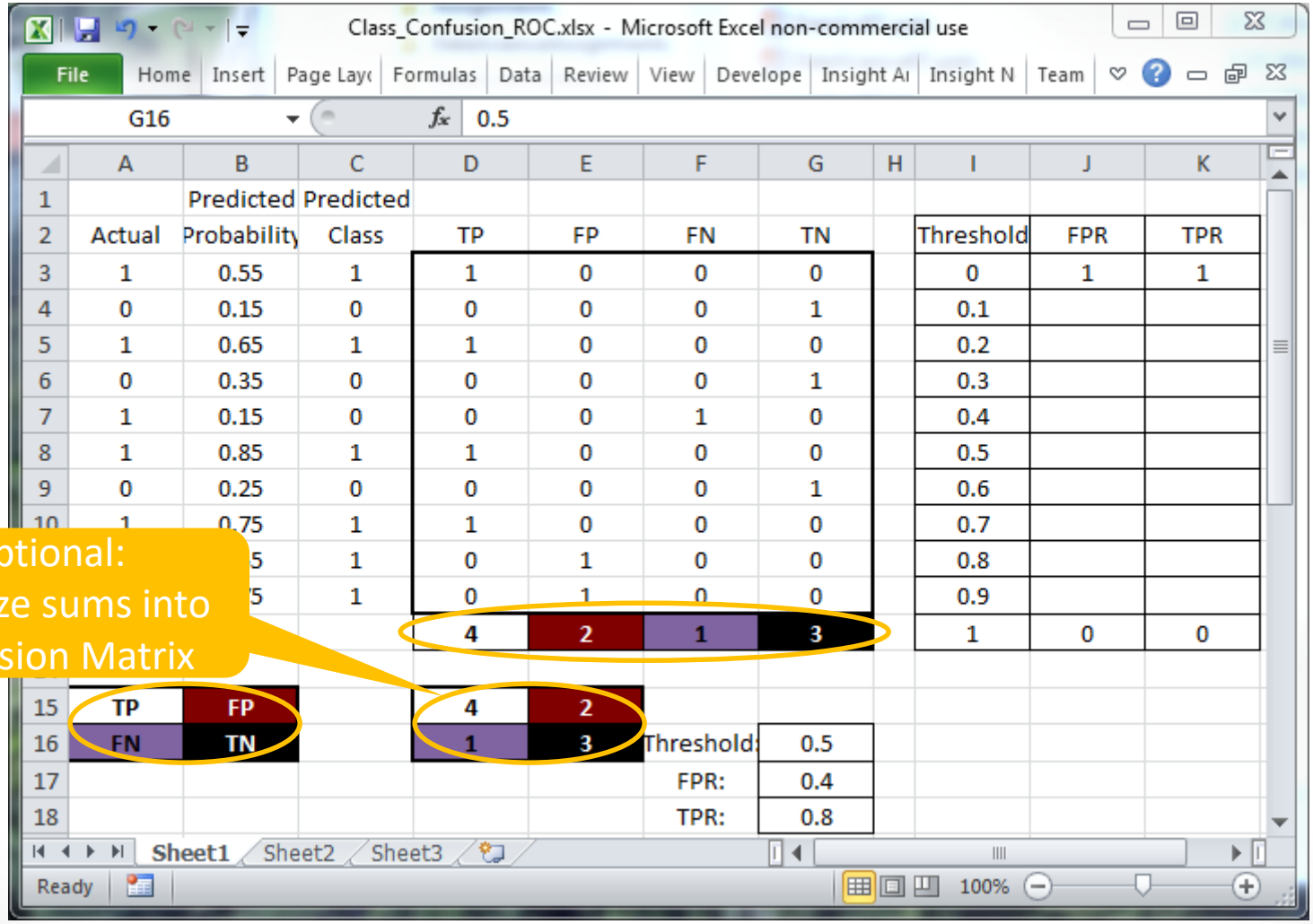


How to make an ROC (9)



	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9			0	0	0	0	1		0.6		
10			1	1	0	0	0		0.7		
11			1	0	1	0	0		0.8		
12			1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3						
17											
18											

How to make an ROC (10)



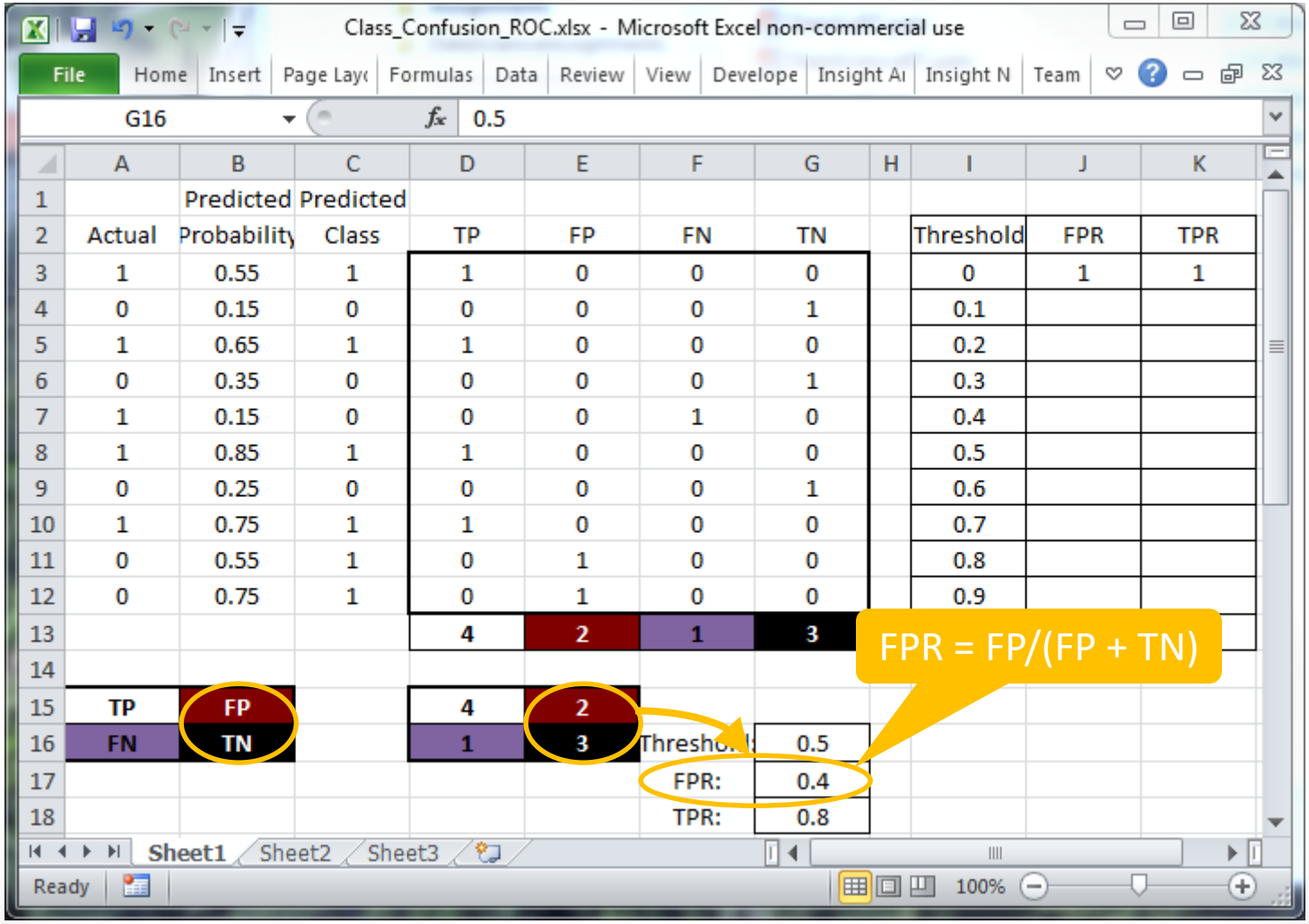
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
		5	1	0	1	0	0		0.8		
		5	1	0	1	0	0		0.9		
				4	2	1	3		1	0	0

TP	FP
FN	TN

4	2
1	3

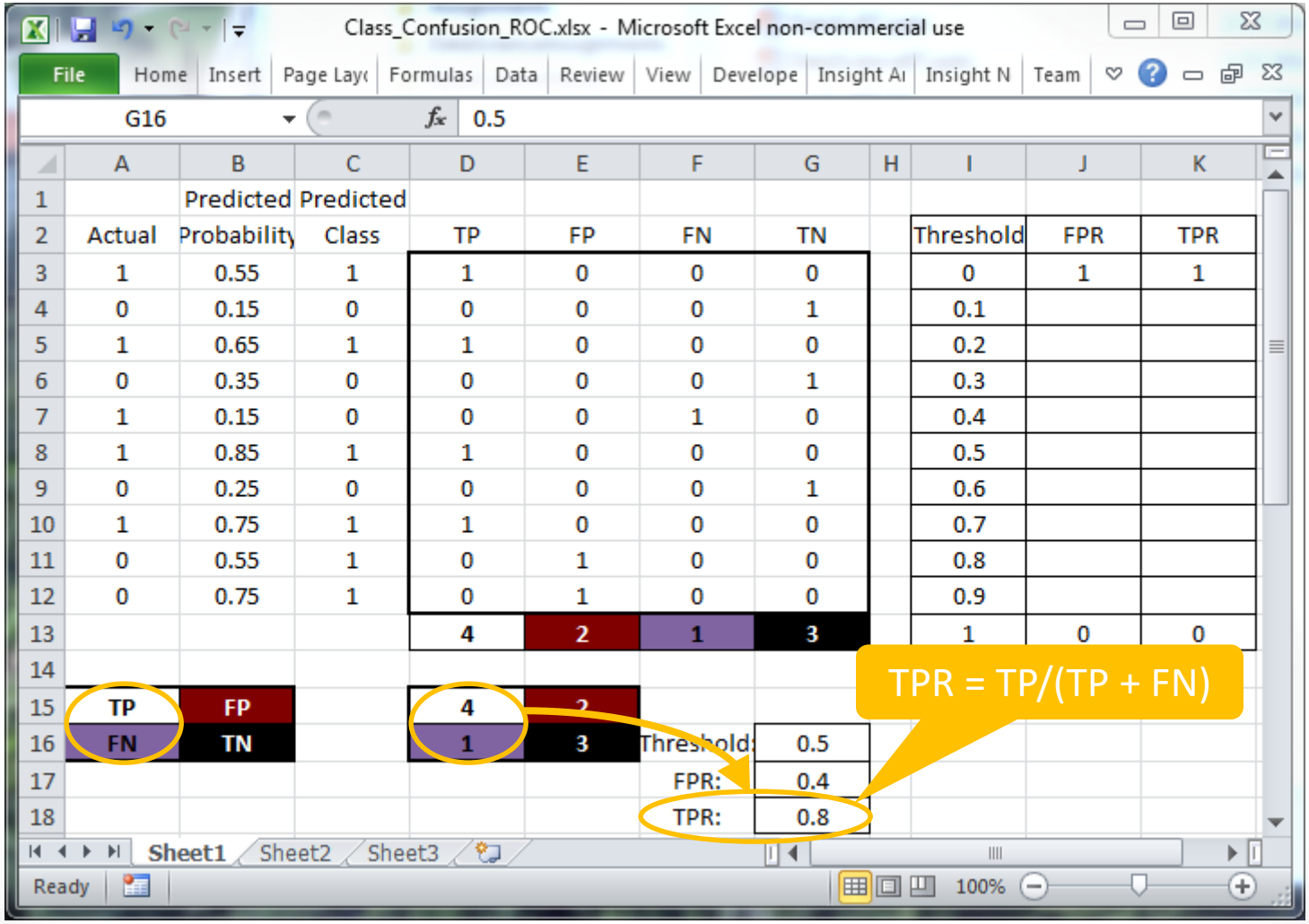
Threshold:	0.5
FPR:	0.4
TPR:	0.8

How to make an ROC (11)



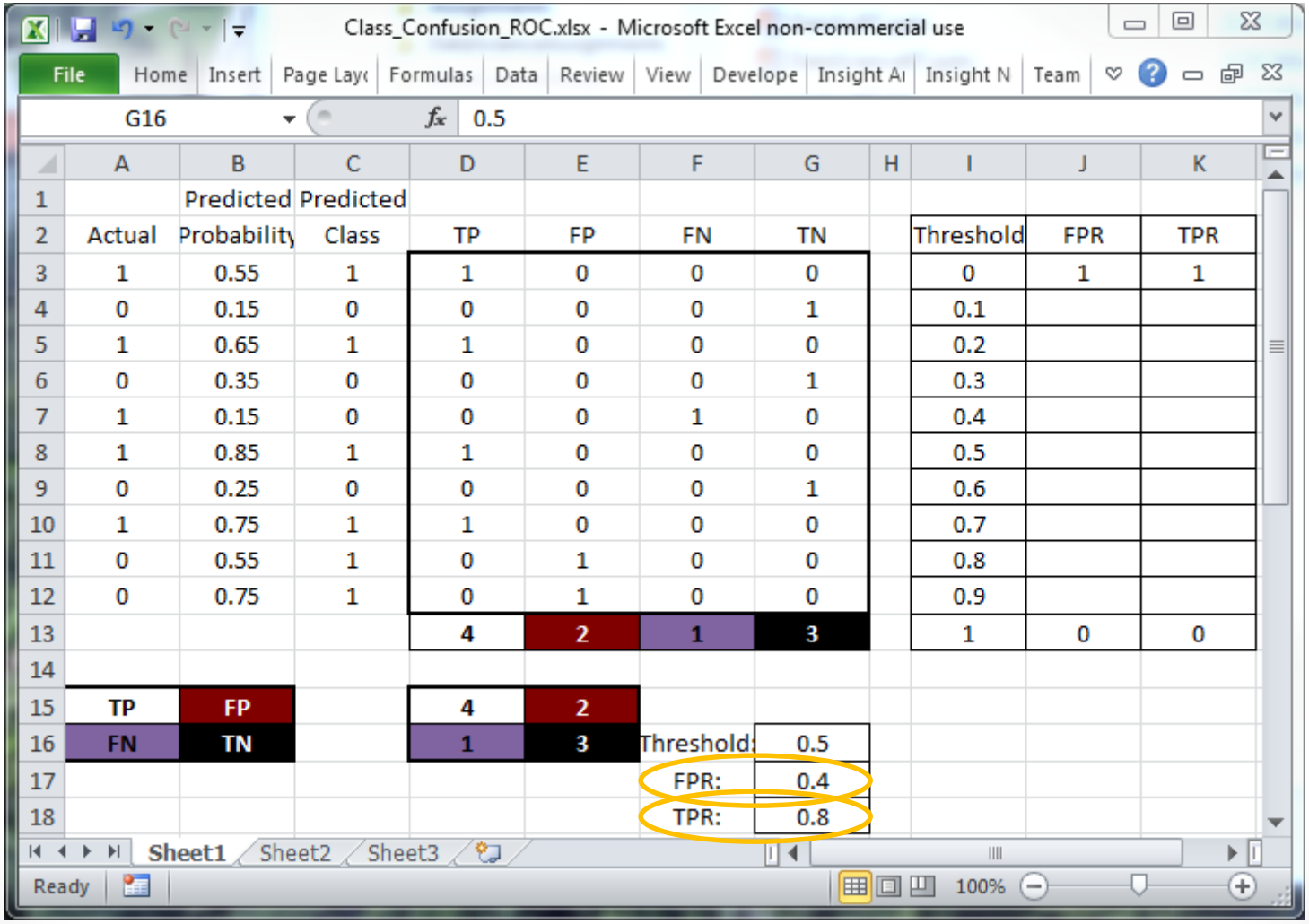
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3				
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (12)



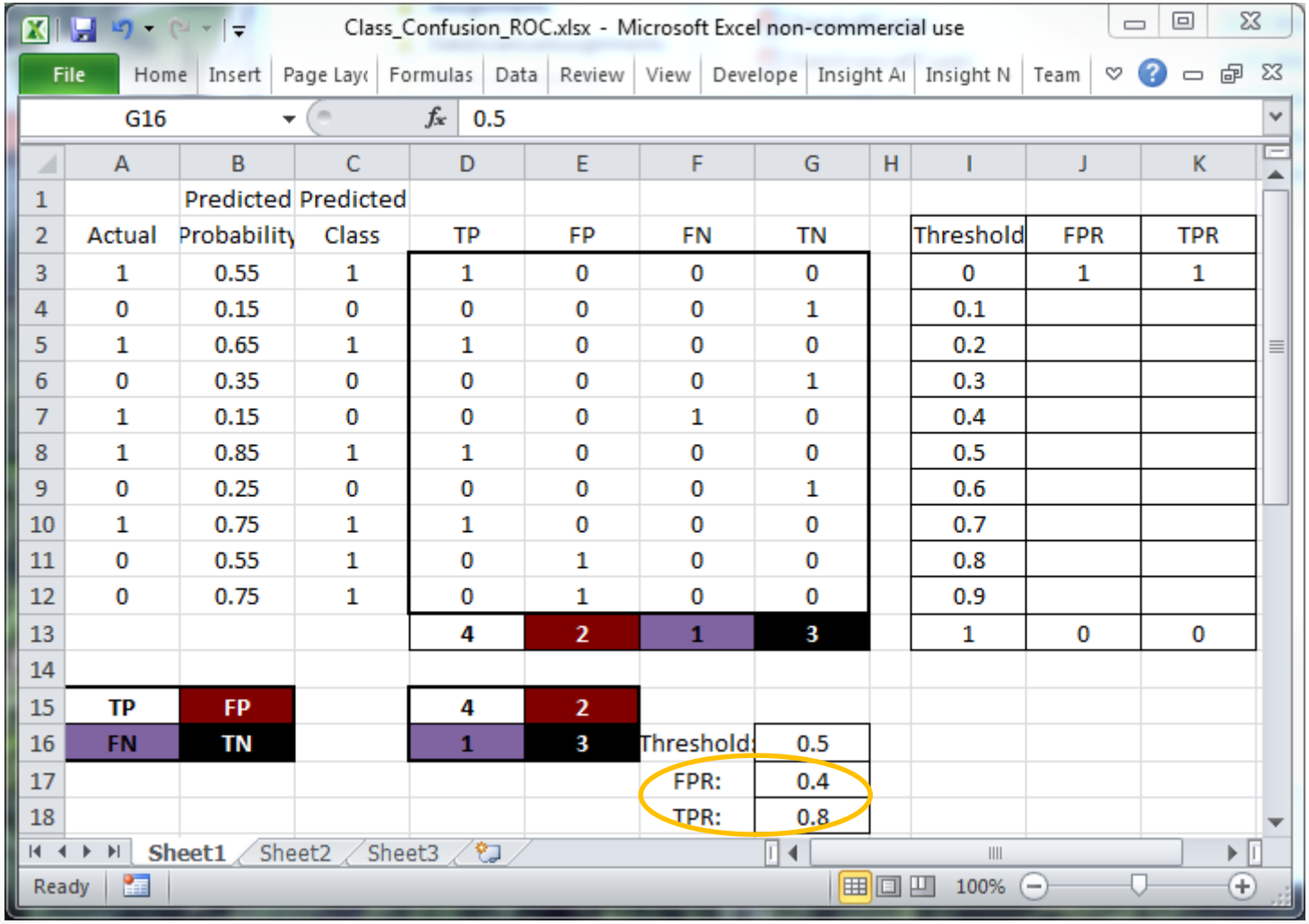
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (13)



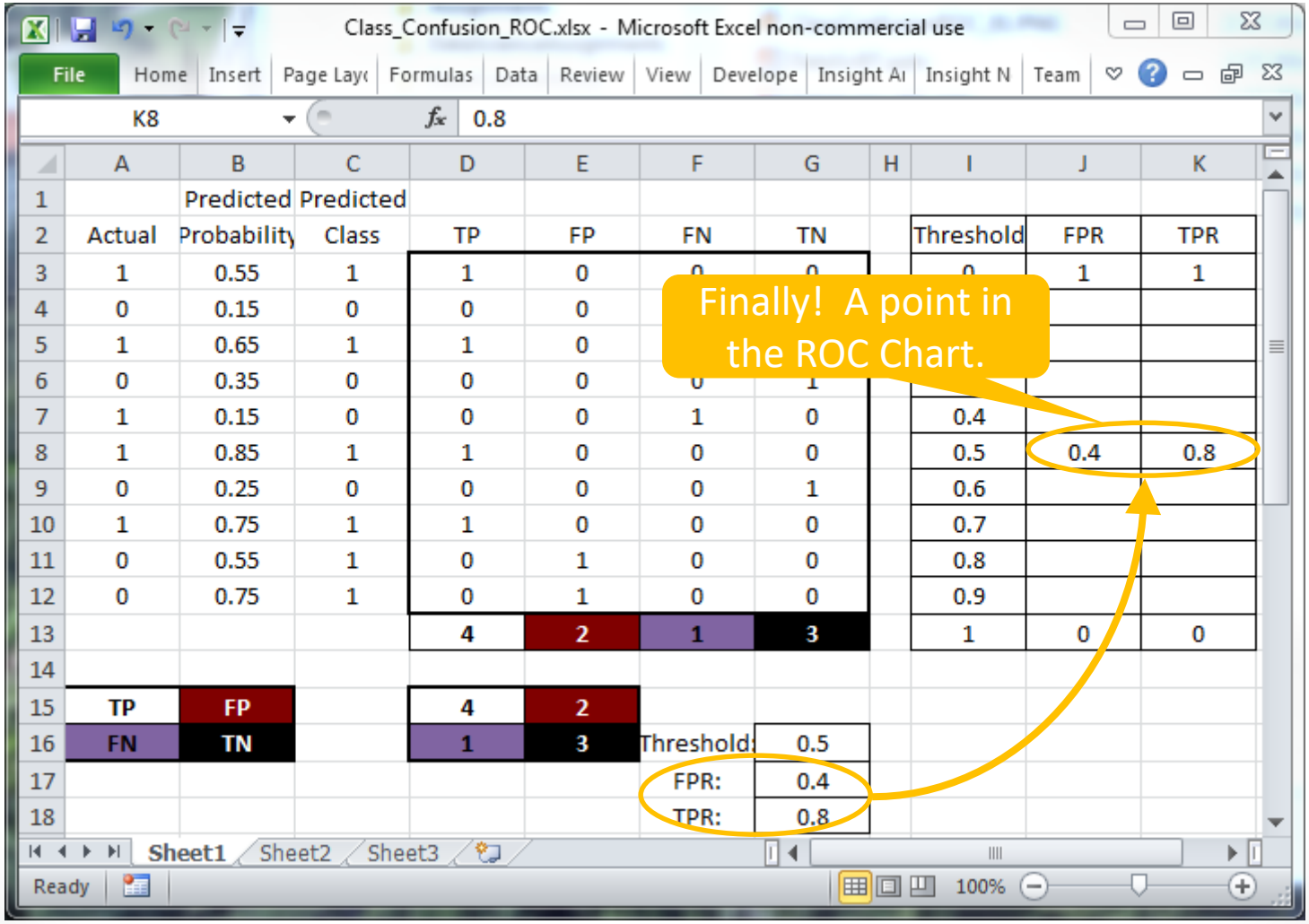
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (14)



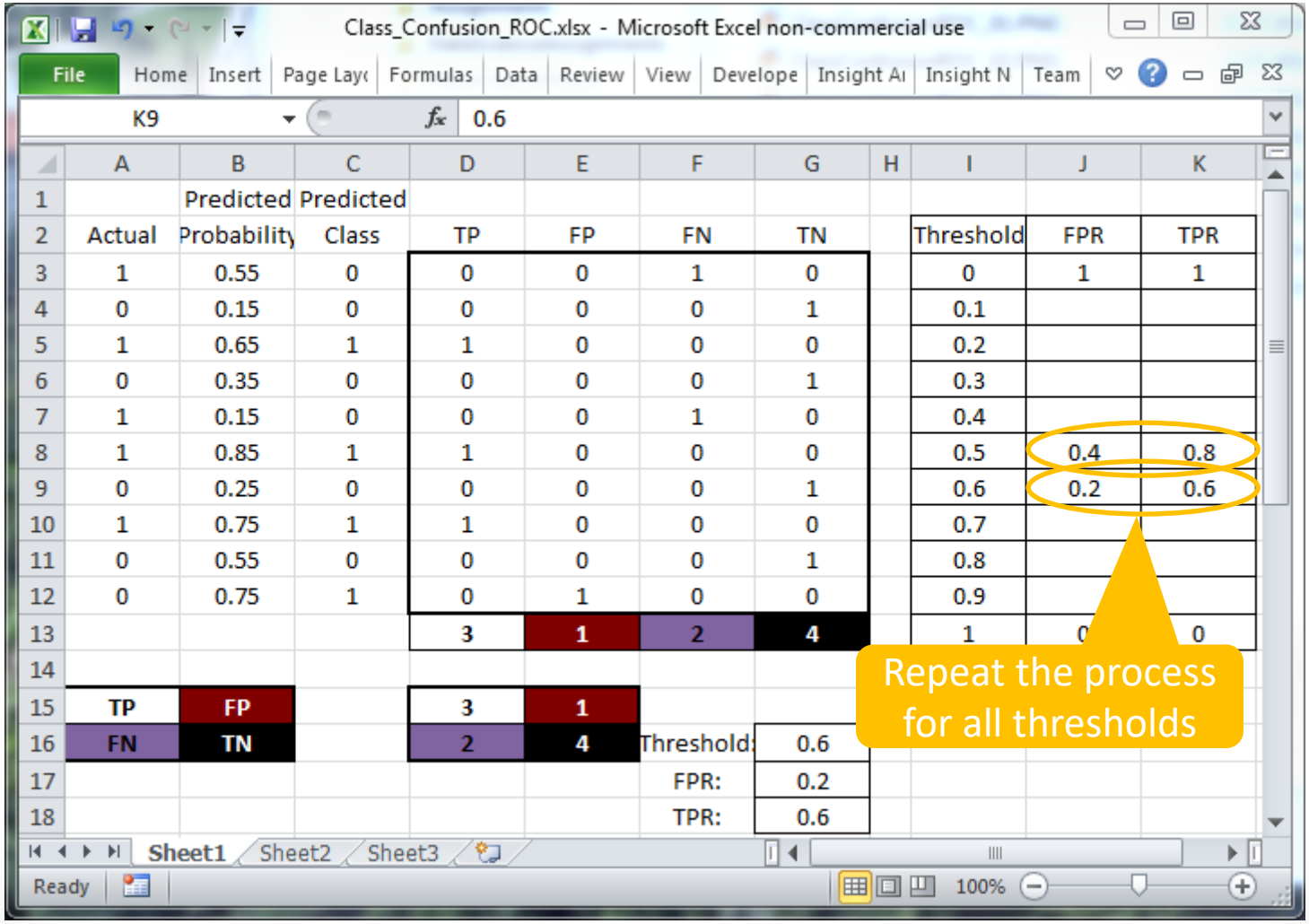
	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5		
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (15)



	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	1	1	0	0	0		0	1	1
4	0	0.15	0	0	0						
5	1	0.65	1	1	0						
6	0	0.35	0	0	0	0	1				
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5	0.4	0.8
9	0	0.25	0	0	0	0	1		0.6		
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	1	0	1	0	0		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				4	2	1	3		1	0	0
14											
15	TP	FP		4	2						
16	FN	TN		1	3	Threshold:	0.5				
17						FPR:	0.4				
18						TPR:	0.8				

How to make an ROC (16)

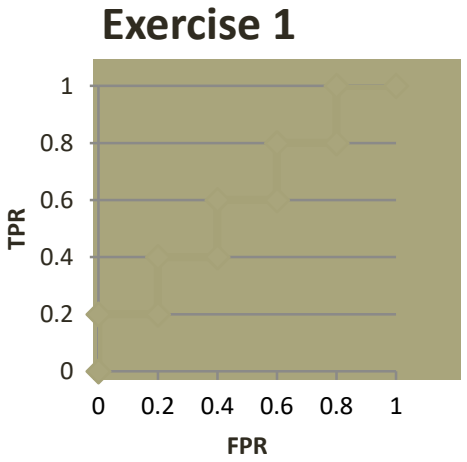


	A	B	C	D	E	F	G	H	I	J	K
1		Predicted	Predicted								
2	Actual	Probability	Class	TP	FP	FN	TN		Threshold	FPR	TPR
3	1	0.55	0	0	0	1	0		0	1	1
4	0	0.15	0	0	0	0	1		0.1		
5	1	0.65	1	1	0	0	0		0.2		
6	0	0.35	0	0	0	0	1		0.3		
7	1	0.15	0	0	0	1	0		0.4		
8	1	0.85	1	1	0	0	0		0.5	0.4	0.8
9	0	0.25	0	0	0	0	1		0.6	0.2	0.6
10	1	0.75	1	1	0	0	0		0.7		
11	0	0.55	0	0	0	0	1		0.8		
12	0	0.75	1	0	1	0	0		0.9		
13				3	1	2	4		1	0	0
14											
15	TP	FP		3	1						
16	FN	TN		2	4	Threshold:	0.6				
17						FPR:	0.2				
18						TPR:	0.6				

How to make an ROC (17)

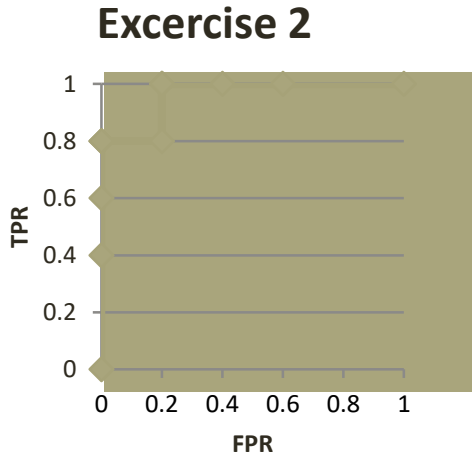
Actual	Predicted Probability
1	0.55
0	0.15
1	0.65
0	0.35
1	0.15
1	0.85
0	0.25
1	0.75
0	0.55
0	0.75

FPR	TPR
1	1
0	0



Actual	Predicted Probability
0	0.15
0	0.25
0	0.35
1	0.45
0	0.45
1	0.55
0	0.65
1	0.75
0	0.85
1	0.95

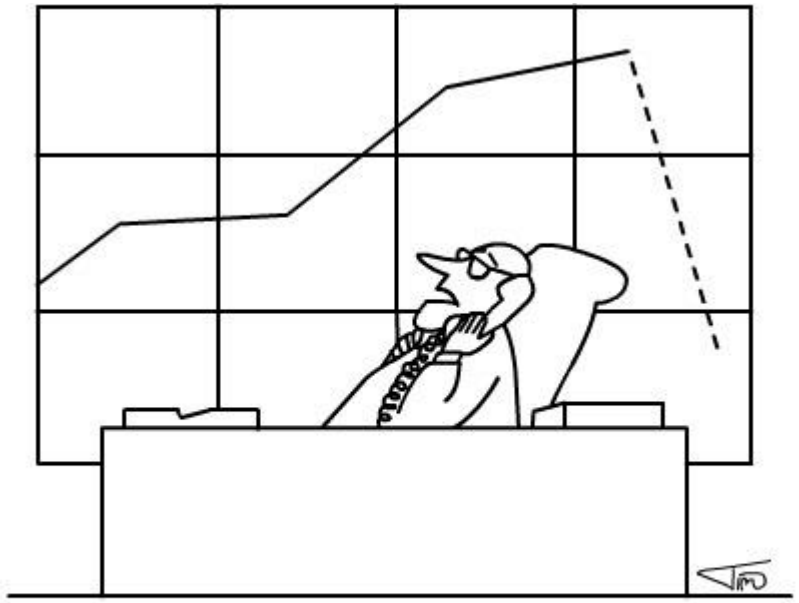
FPR	TPR
1	1
0	0



How to make an ROC

Break

- Documentaries on Predictive Analytics:
  - https://www.analyticsvidhya.com/blog/2015/11/7-watch-documentaries-statistics-machine-learning/

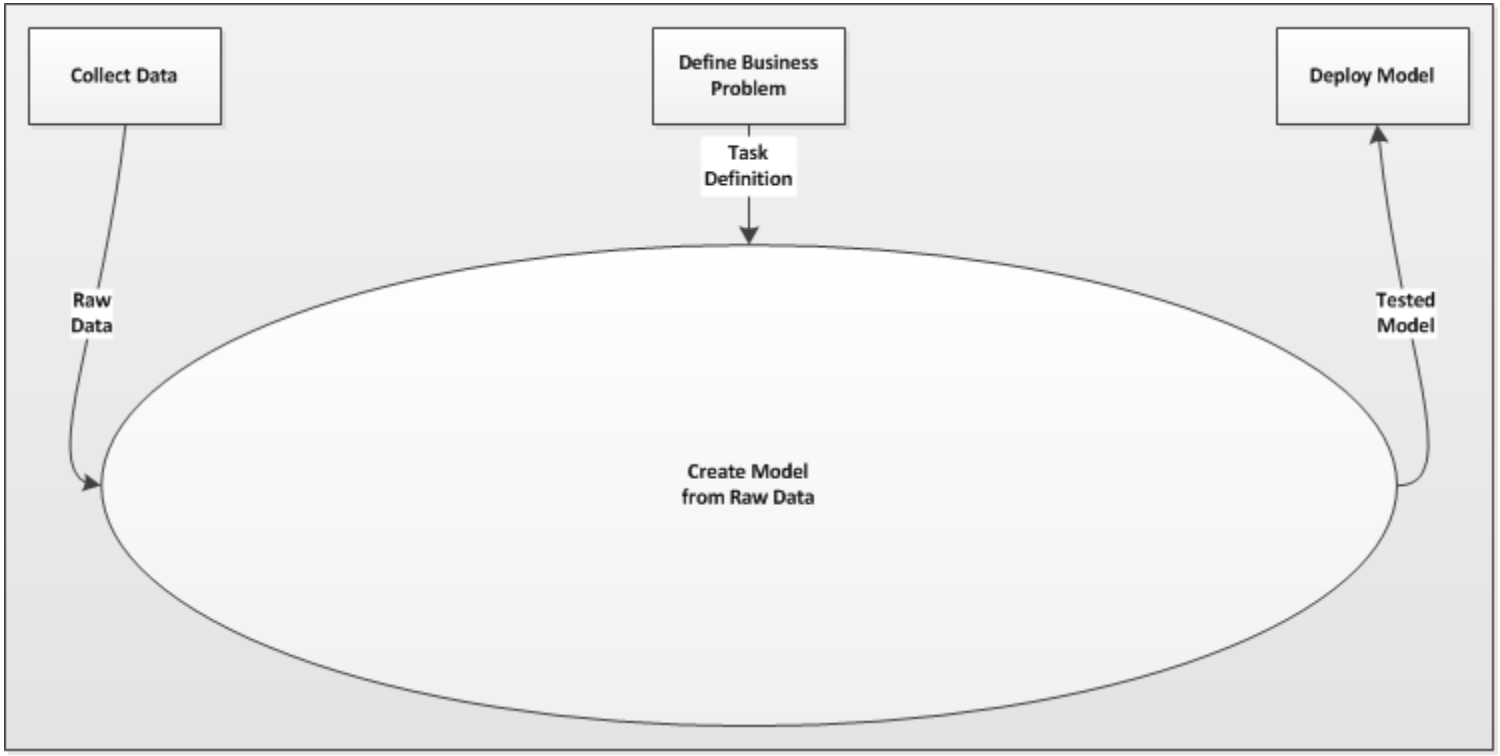


"BI tech support? The predictive analysis system is giving the wrong answer again—can you please fix it?... "

Modeling Iteration Trap

The problem with iterative data preparation and training refinements

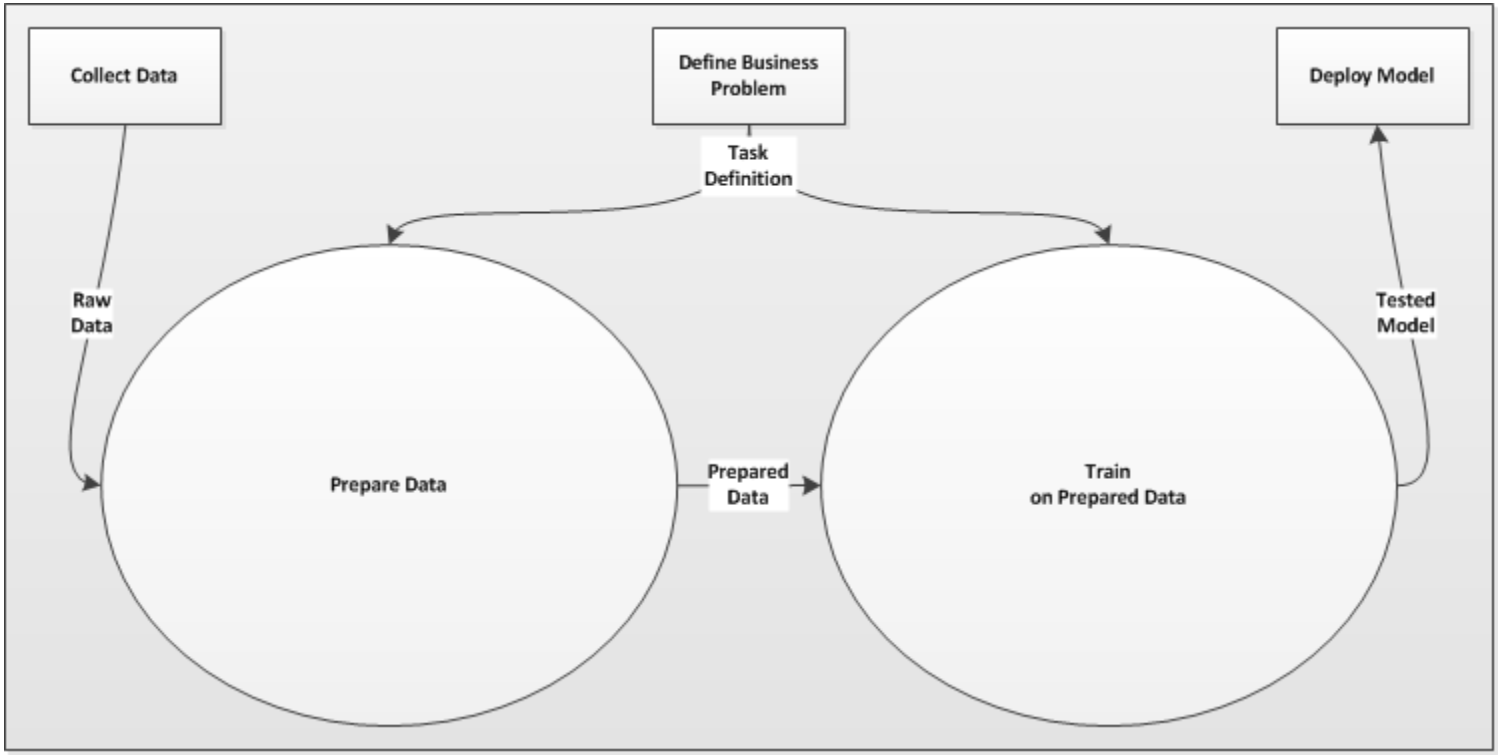
Modeling Iteration Trap (0)



Basic Predictive Analytics

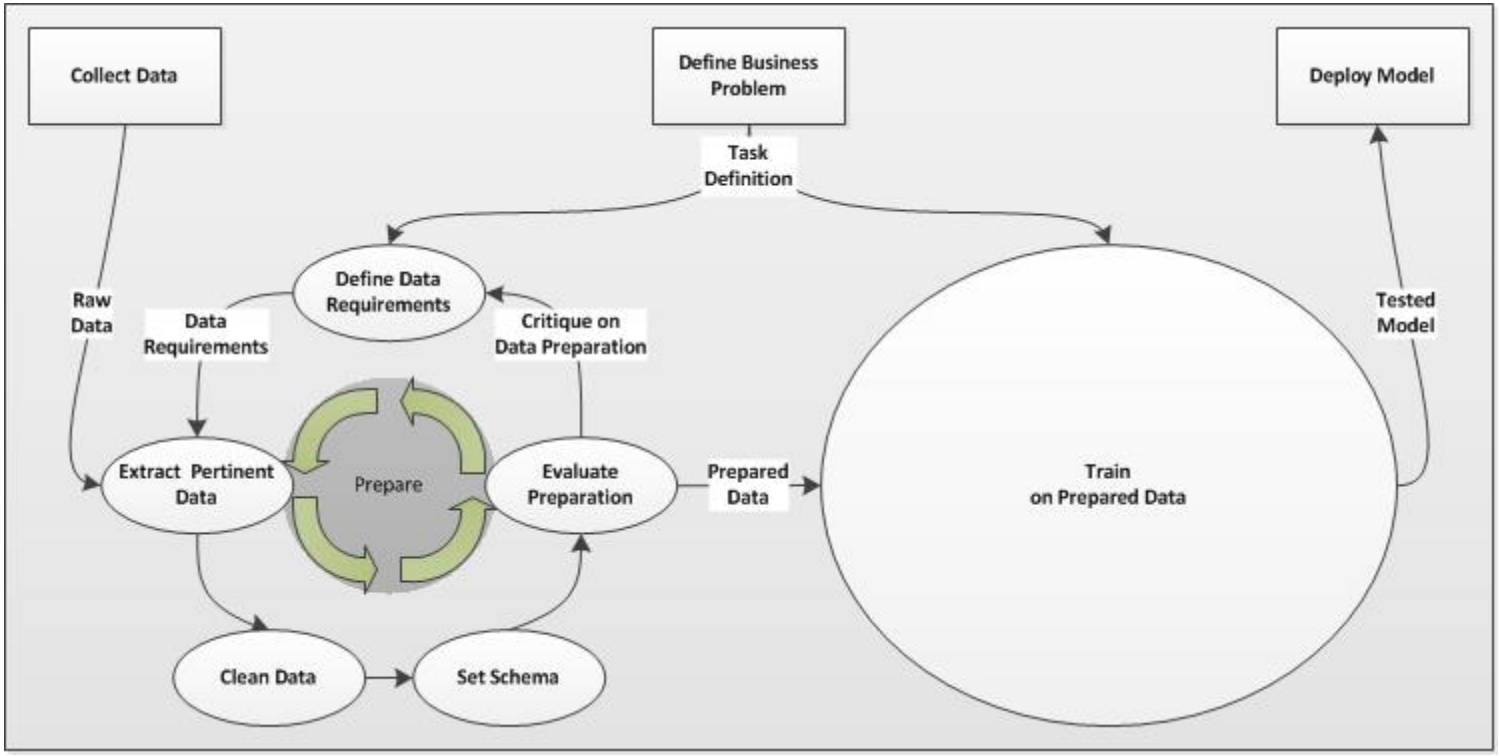
L0-DFD

Modeling Iteration Trap (1)



Predictive Analytics consists of Data Preparation and Modeling
L1-DFD

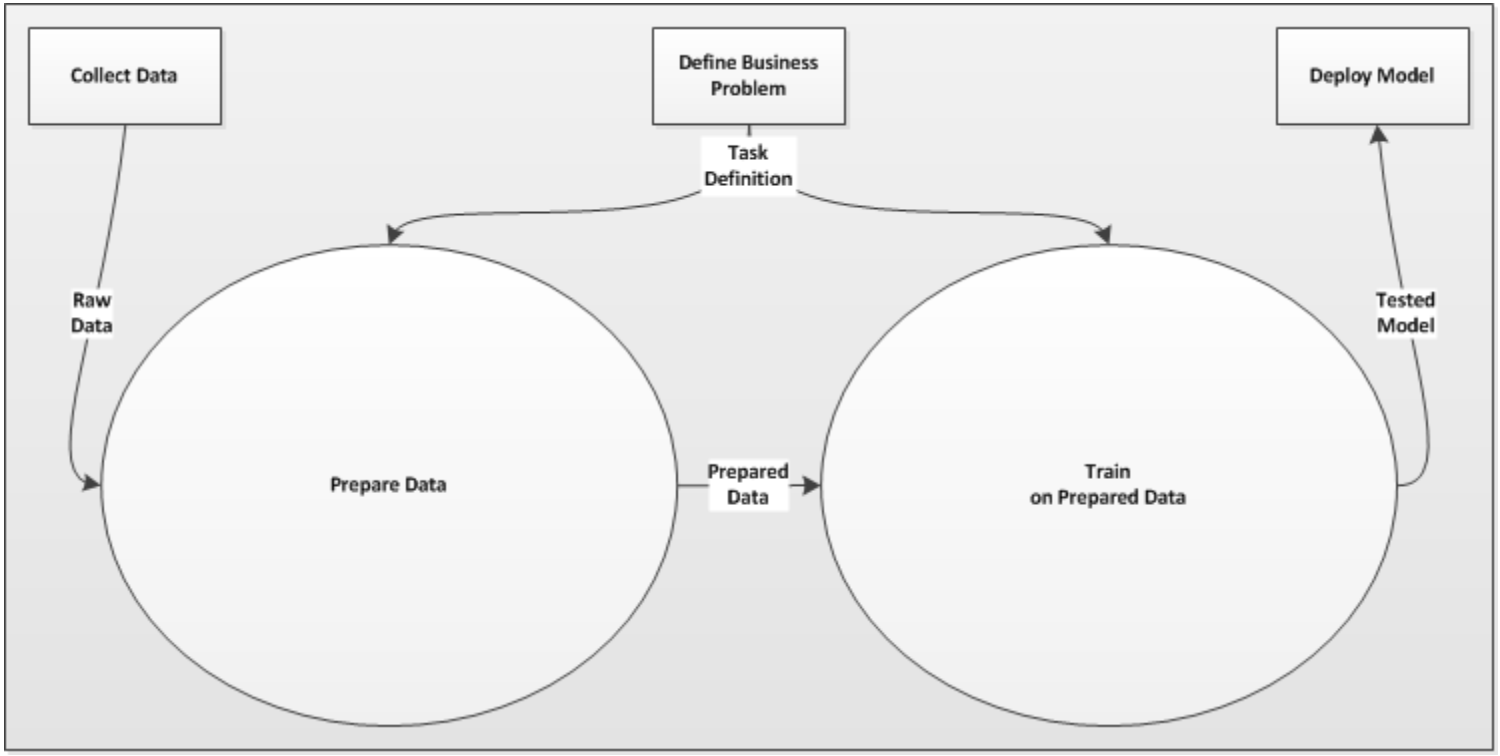
Modeling Iteration Trap (2)



Data Preparation is Iterative

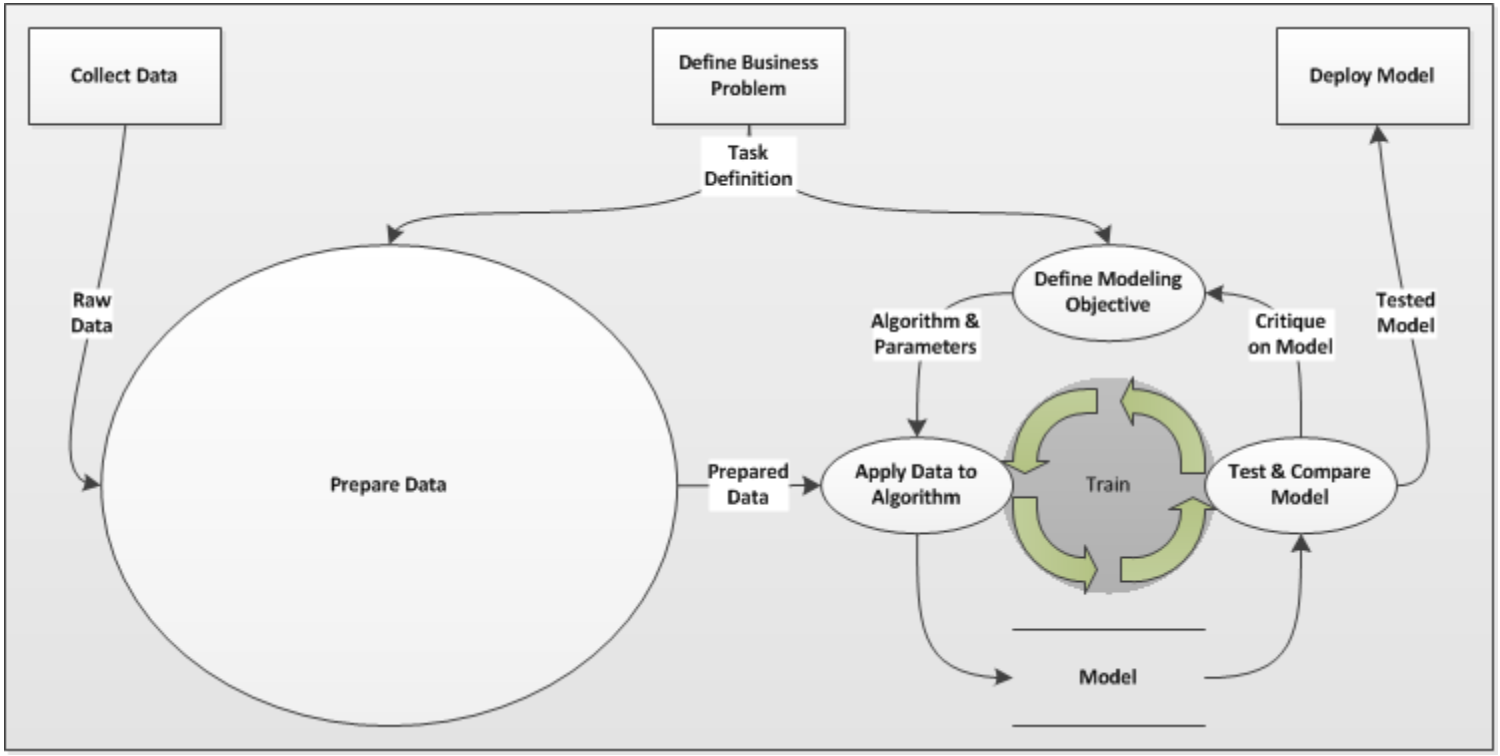
L2-DFD

Modeling Iteration Trap (3)



Predictive Analytics consists of Data Preparation and Modeling
L1-DFD

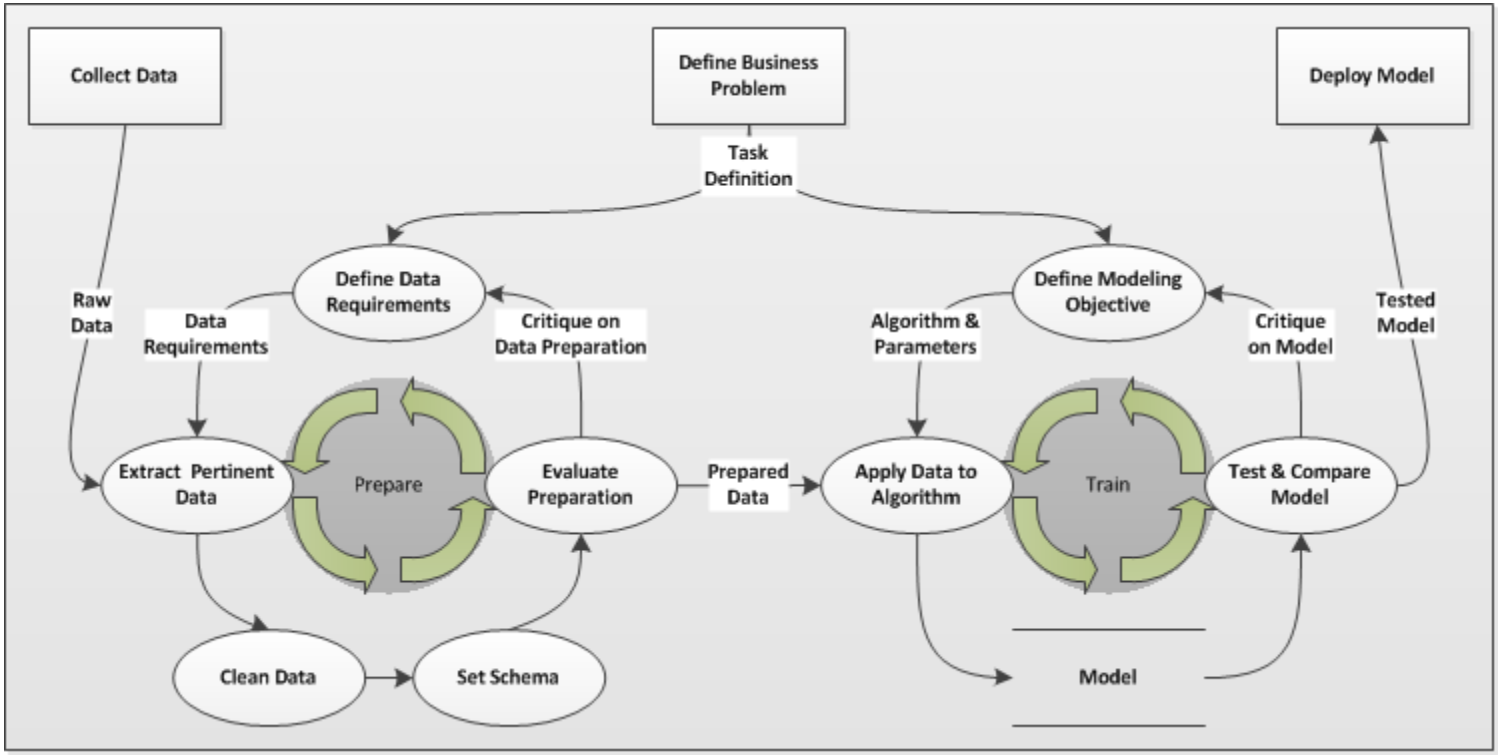
Modeling Iteration Trap (4)



Training is Iterative

L2-DFD

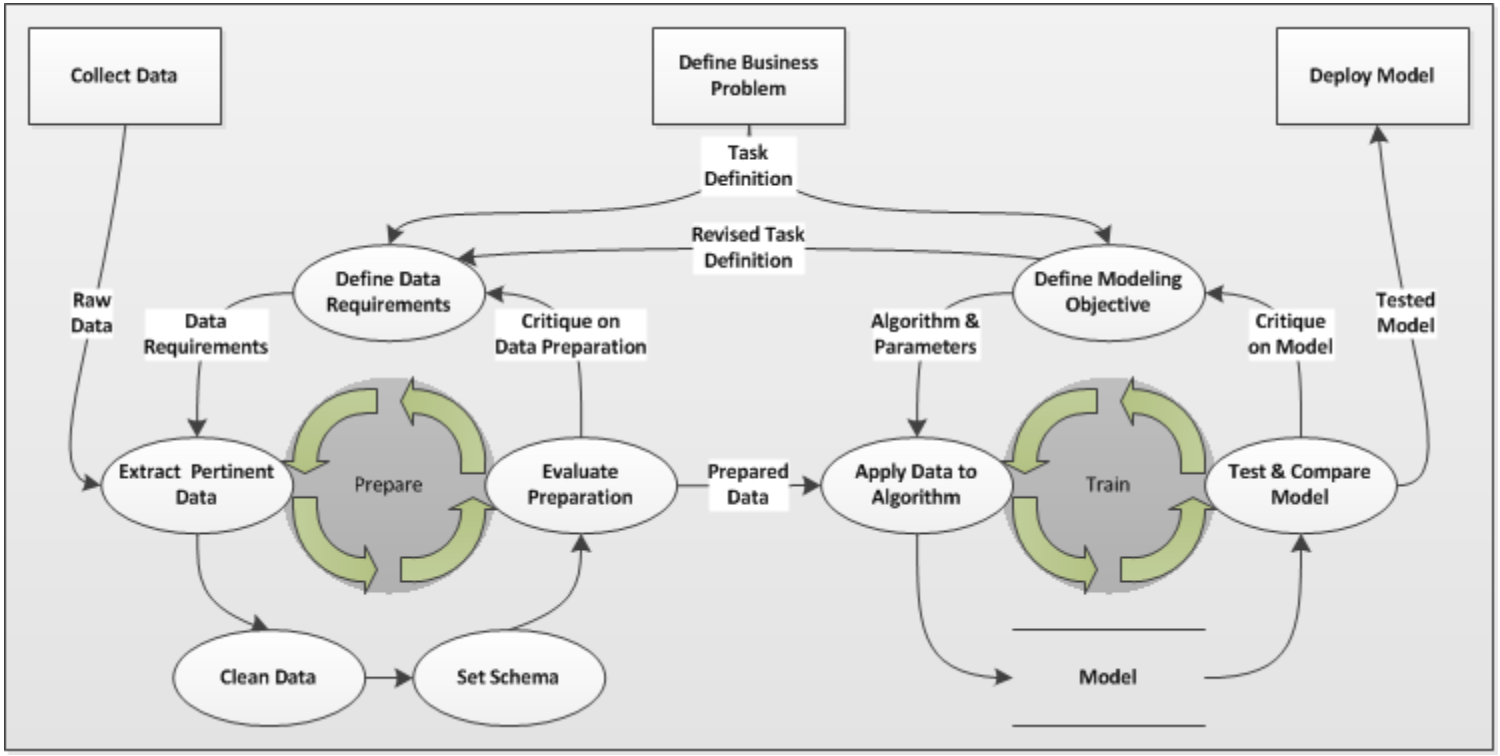
Modeling Iteration Trap (5)



Data Preparation and Training

L2-DFD

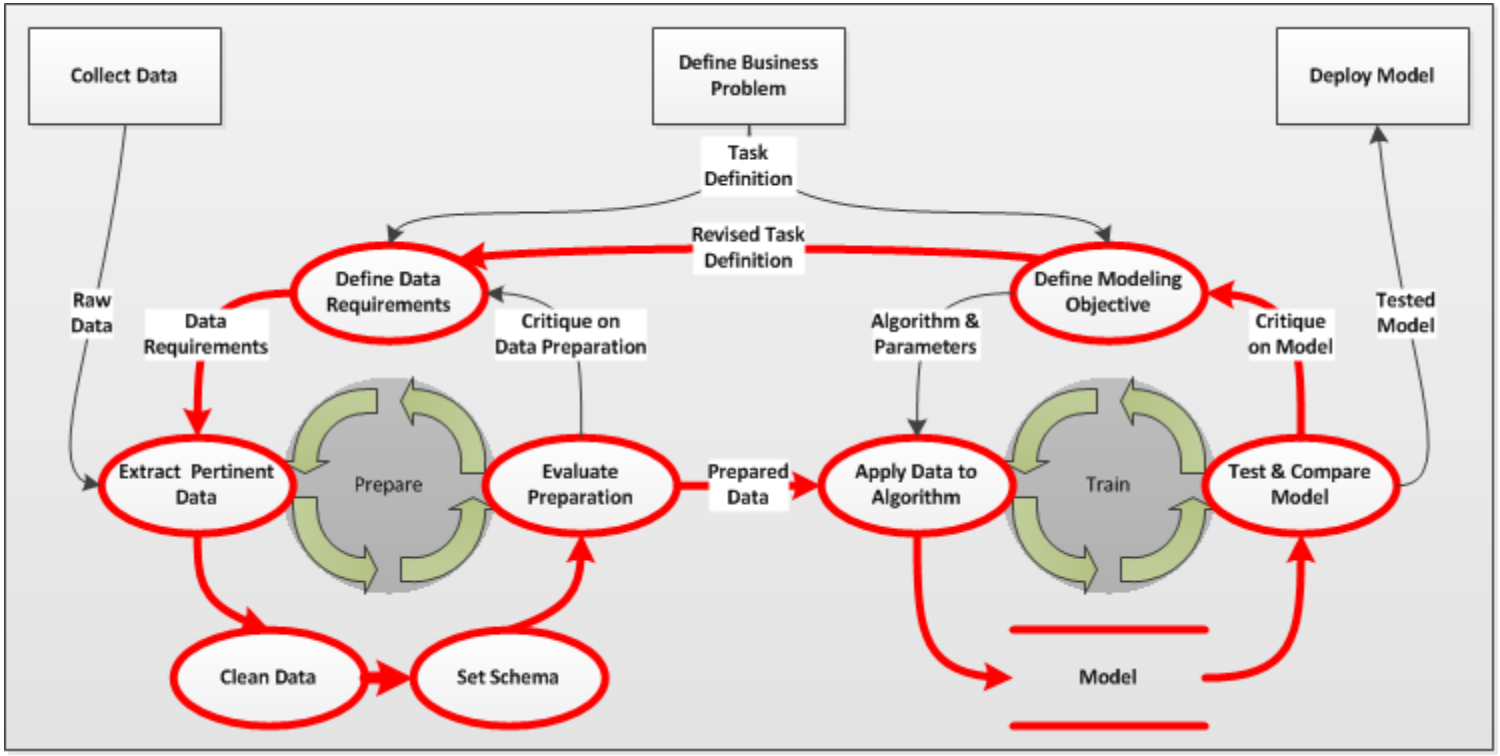
Modeling Iteration Trap (6)



Modeling Revises the Task Definition

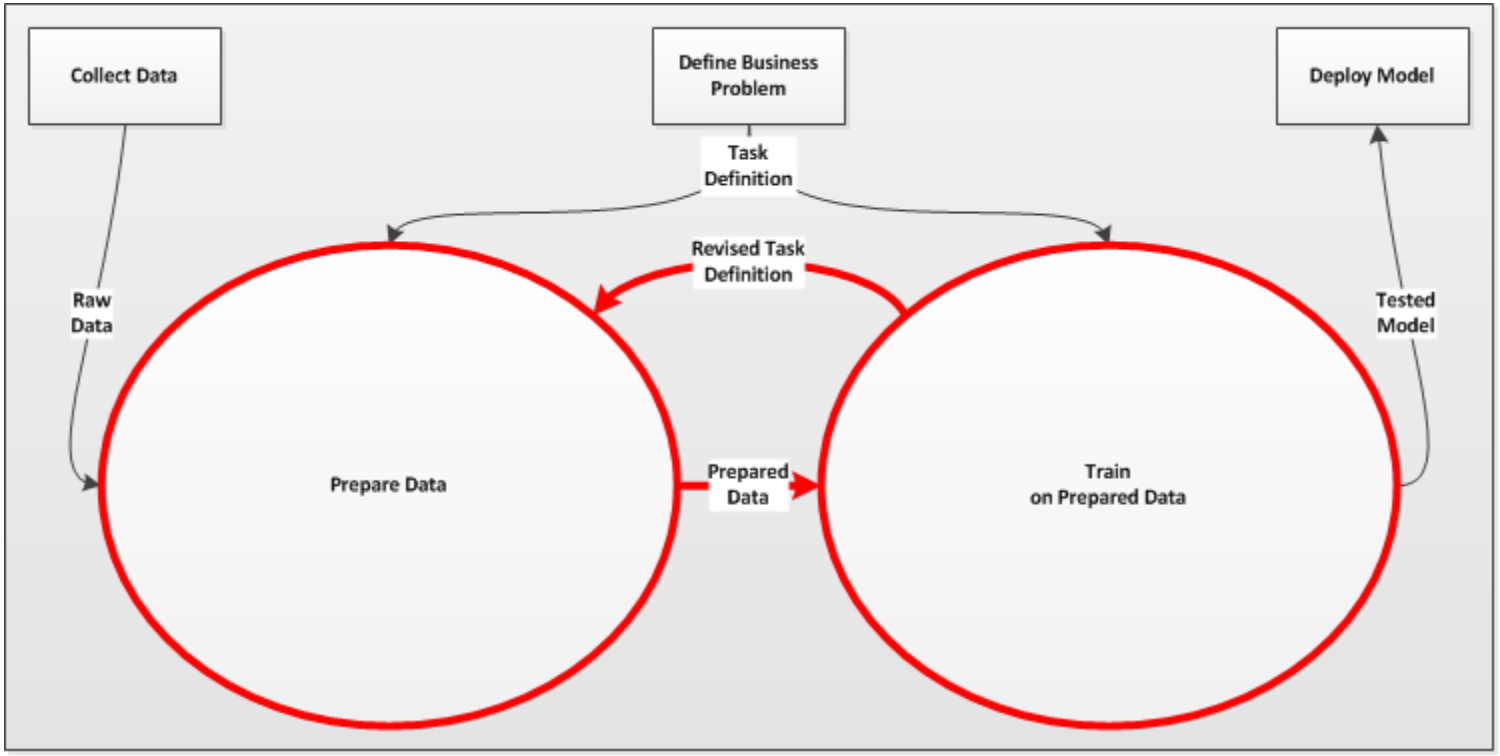
L2-DFD

Modeling Iteration Trap (7)



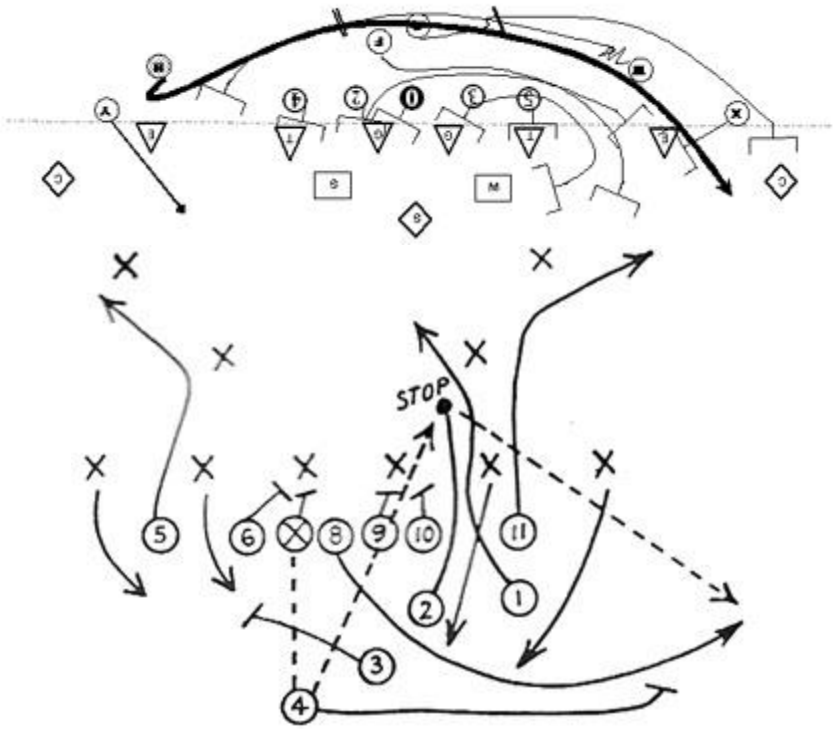
Revised Task Definition Completes a Cycle that is hard to optimize. Engineers get caught in a loop.

Modeling Iteration Trap (8)



Revised Task Definition Completes a Cycle that is hard to optimize. Engineers get caught in a loop.

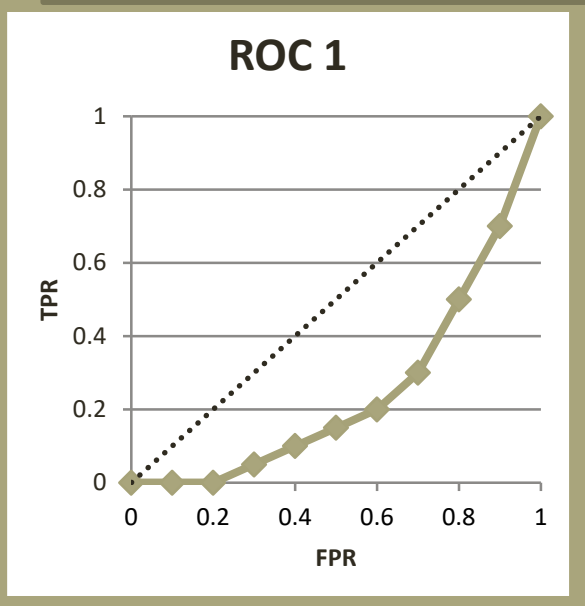
Modeling Iteration Trap (9)

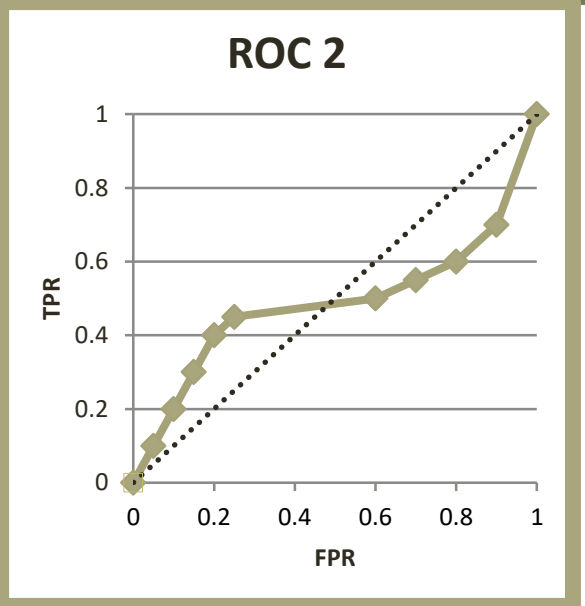


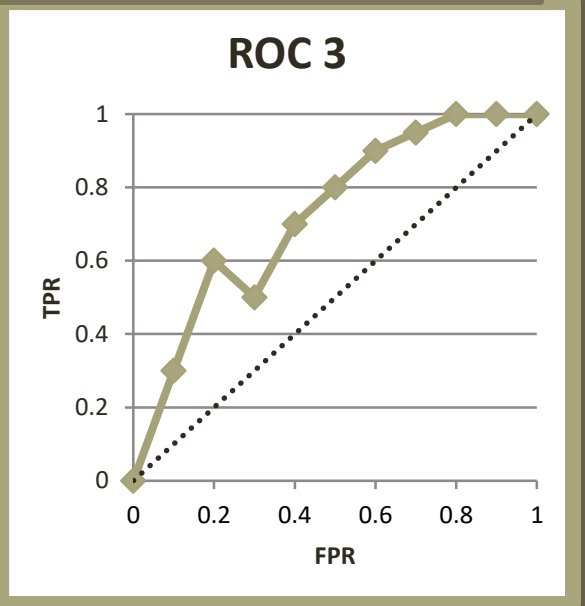
Modeling Iteration Trap

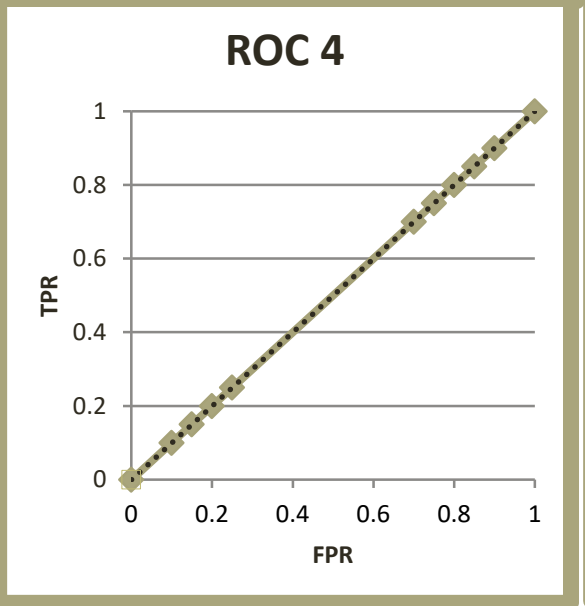
The problem with iterative data preparation and training refinements

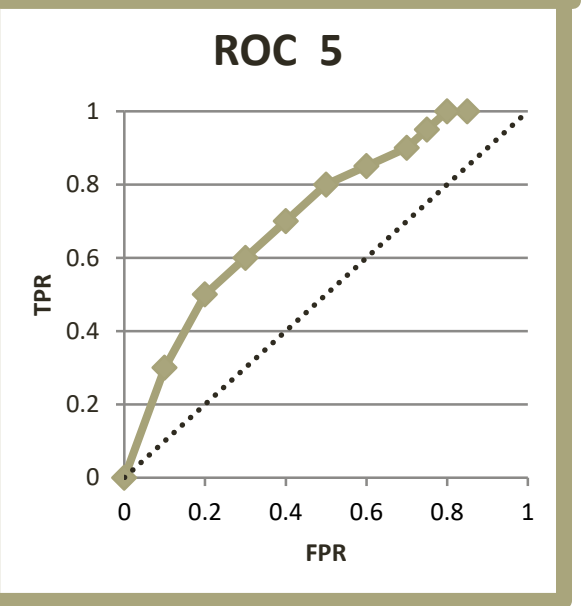
Lesson 09 Quiz 1 Question 9: Which ROC curves are incorrect?











Review Terminology

- Algorithm
- Anomaly detection
- Association
- Attribute
- Binarize Categories
- Binary Column
- Case
- Category Column
- Character Column
- Classification
- Clustering
- Coercion
- Column
- Column Header
- Confusion Matrix
- Data
- Data Dimensionality
- Data Frame
- Data Type
- DFD
- Dummy Variable
- Estimation
- False Positive
- False Negative
- Feature Scaling
- Field
- Hypothesis
- Key Column
- Machine Learning
- Market-basket analysis
- Matrix
- Missing Data
- Model
- Multinomial Column
- Normalization
- Numeric Column
- Observation
- One-hot encoding
- Outcome
- Outlier Removal
- Predictive Analytics
- Rectangular Data
- Relabeling
- ROC curve
- Row
- Schema
- Shaping Data
- Sparse Multi-Dimensional Matrix
- Standard Deviation
- States
- String
- Supervised Learning
- Support
- Table
- Target Column
- Text Column
- Theory
- Un-structured Data
- Unsupervised Learning
- Z-score

Introduction to Data Science