



Deep Learning for Healthcare

3. Machine Learning Basics

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Evaluation metrics



- Metrics for classification tasks
- Metrics for regression tasks
- Metrics for clustering tasks
- Evaluation strategy

Performance Metrics: Classification



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative

Performance Metrics: Classification



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative

Prediction	Prediction Outcome Positive
	Prediction Outcome Negative

Performance Metrics: Classification



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative

Ground Truth	
Condition Positive	Condition Negative

Performance Metrics: Classification



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative

True Positive

Performance Metrics: Classification



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative

False Positive
(Type I error)

Performance Metrics: Classification



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative

False Negative
(Type II error)

Performance Metrics: Classification



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative

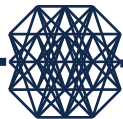
True Negative

Performance Metrics: Classification



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative

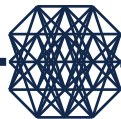
Confusion Matrix Quiz



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	TOTAL POPULATION	<input type="text"/>	935
	Prediction Outcome Positive	True Positive <input type="text"/>	False Positive 100
	Prediction Outcome Negative	False Negative 10	True Negative <input type="text"/>

Please fill in the
missing numbers.

Confusion Matrix Quiz



		Ground Truth	
		Condition Positive	Condition Negative
Prediction	TOTAL POPULATION 1000	65	935
	Prediction Outcome Positive 155	True Positive 55	False Positive 100
	Prediction Outcome Negative 845	False Negative 10	True Negative 835

Please fill in the
missing numbers.

Performance Metrics: Classification



		Ground Truth	
TOTAL POPULATION		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False Positive}}{\text{Condition negative}}$
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$

Performance Metrics: Classification



		Ground Truth	
TOTAL POPULATION		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False positive}}{\text{Condition negative}}$
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$

$$\begin{aligned} &\text{True Positive Rate} \\ &(\text{Sensitivity, Recall}) \\ &= \\ &\frac{\text{True positive}}{\text{Condition positive}} \end{aligned}$$

PERFORMANCE METRICS: CLASSIFICATION



		Ground Truth	
TOTAL POPULATION		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False positive}}{\text{Condition negative}}$
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$

$$\text{False Negative Rate} = \frac{\text{False negative}}{\text{Condition positive}}$$

Performance Metrics: Classification



		Ground Truth	
TOTAL POPULATION		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False Positive}}{\text{Condition negative}}$
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$

$$\text{False Positive Rate} = \frac{\text{False Positive}}{\text{Condition negative}}$$

Performance Metrics: Classification



		Ground Truth	
TOTAL POPULATION		Condition Positive	Condition Negative
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)
	Prediction Outcome Negative	False Negative (Type II error)	True Negative
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False positive}}{\text{Condition negative}}$
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate (Specificity) = $\frac{\text{True negative}}{\text{Condition negative}}$

$$\begin{aligned} &\text{True Negative Rate} \\ &\text{(Specificity)} \\ &= \\ &\frac{\text{True negative}}{\text{Condition negative}} \end{aligned}$$

Accuracy Metrics Quiz



		Ground Truth	
TOTAL POPULATION 1000		Condition Positive 65	Condition Negative 935
Prediction	Prediction Outcome Positive 155	True Positive 55	False Positive 100
	Prediction Outcome Negative 845	False Negative 10	True Negative 835
Accuracy 89%		True Positive Rate <input type="text"/>	False Positive Rate <input type="text"/>
		False Negative Rate <input type="text"/>	True Negative Rate <input type="text"/>

Please fill in the
missing numbers.

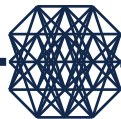
ACCURACY METRICS QUIZ



		Ground Truth	
TOTAL POPULATION 1000		Condition Positive 65	Condition Negative 935
Prediction	Prediction Outcome Positive 155	True Positive 55	False Positive 100
	Prediction Outcome Negative 845	False Negative 10	True Negative 835
Accuracy 89%		True Positive Rate 85%	False Positive Rate 11%
		False Negative Rate 15%	True Negative Rate 89%

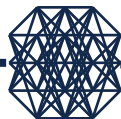
Please fill in the
missing numbers.

Performance Metrics: Classification



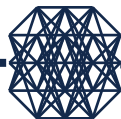
		Ground Truth			
TOTAL POPULATION		Condition Positive	Condition Negative	Prevalence $= \frac{\text{Condition Positive}}{\text{Total population}}$	
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)	Positive Predictive Value $= \frac{\text{True Positive}}{\text{Prediction outcome positive}}$	False Discovery Rate $= \frac{\text{False Positive}}{\text{Prediction outcome positive}}$
	Prediction Outcome Negative	False Negative (Type II error)	True Negative	False Omission Rate $= \frac{\text{False negative}}{\text{Prediction outcome negative}}$	Negative Predictive Value $= \frac{\text{True negative}}{\text{Prediction outcome negative}}$
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate $= \frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate $= \frac{\text{False Positive}}{\text{Condition negative}}$	Prevalence $= \frac{\text{Condition Positive}}{\text{Total population}}$	
		False Negative Rate $= \frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate $= \frac{\text{True negative}}{\text{Condition negative}}$		

Performance Metrics: Classification



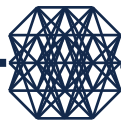
		Ground Truth			
TOTAL POPULATION		Condition Positive	Condition Negative	Prevalence = $\frac{\text{Condition Positive}}{\text{Total population}}$	
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)	Positive Predictive Value = $\frac{\text{True Positive}}{\text{Prediction outcome positive}}$	False Discovery Rate = $\frac{\text{False Positive}}{\text{Prediction outcome positive}}$
	Prediction Outcome Negative	False Negative (Type II error)	True Negative	False Omission Rate = $\frac{\text{False negative}}{\text{Prediction outcome negative}}$	Negative Predictive Value = $\frac{\text{True negative}}{\text{Prediction outcome negative}}$
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False Positive}}{\text{Condition negative}}$	Positive Predictive Value (Precision) = $\frac{\text{True Positive}}{\text{Test outcome positive}}$	
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$		

Performance Metrics: Classification



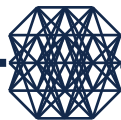
		Ground Truth			
		TOTAL POPULATION	Condition Positive	Condition Negative	Prevalence = $\frac{\text{Condition Positive}}{\text{Total population}}$
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)	Positive Predictive Value = $\frac{\text{True Positive}}{\text{Prediction outcome positive}}$	False Discovery Rate = $\frac{\text{False Positive}}{\text{Prediction outcome positive}}$
	Prediction Outcome Negative	False Negative (Type II error)	True Negative	False Omission Rate = $\frac{\text{False negative}}{\text{Prediction outcome negative}}$	Negative Predictive Value = $\frac{\text{True negative}}{\text{Prediction outcome negative}}$
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False Positive}}{\text{Condition negative}}$	False Discovery Rate = $\frac{\text{False Positive}}{\text{Prediction outcome positive}}$	
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$		

Performance Metrics: Classification



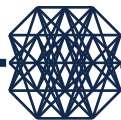
		Ground Truth			
TOTAL POPULATION		Condition Positive	Condition Negative	Prevalence = $\frac{\text{Condition Positive}}{\text{Total population}}$	
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)	Positive Predictive Value = $\frac{\text{True Positive}}{\text{Prediction outcome positive}}$	False Discovery Rate = $\frac{\text{False Positive}}{\text{Prediction outcome positive}}$
	Prediction Outcome Negative	False Negative (Type II error)	True Negative	False Omission Rate = $\frac{\text{False negative}}{\text{Prediction outcome negative}}$	Negative Predictive Value = $\frac{\text{True negative}}{\text{Prediction outcome negative}}$
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False Positive}}{\text{Condition negative}}$	<div> Negative Predictive Value = $\frac{\text{True negative}}{\text{Prediction outcome negative}}$ </div>	
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$		

Performance Metrics: Classification



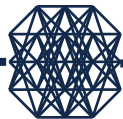
		Ground Truth			
		TOTAL POPULATION	Condition Positive	Condition Negative	Prevalence = $\frac{\text{Condition Positive}}{\text{Total population}}$
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)	Positive Predictive Value = $\frac{\text{True Positive}}{\text{Prediction outcome positive}}$	False Discovery Rate = $\frac{\text{False Positive}}{\text{Prediction outcome positive}}$
	Prediction Outcome Negative	False Negative (Type II error)	True Negative	False Omission Rate = $\frac{\text{False negative}}{\text{Prediction outcome negative}}$	Negative Predictive Value = $\frac{\text{True negative}}{\text{Prediction outcome negative}}$
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False Positive}}{\text{Condition negative}}$	False Omission Rate = $\frac{\text{False negative}}{\text{Prediction outcome negative}}$	
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$		

Predictive Metrics Quiz



		Ground Truth			
		TOTAL POPULATION 1000	Condition Positive 65	Condition Negative 935	Prevalence <input type="text"/>
Prediction	Prediction Outcome Positive 155	True Positive 55	False Positive 100	Positive Predictive Value <input type="text"/>	False Discovery Rate <input type="text"/>
	Prediction Outcome Negative 845	False Negative 10	True Negative 835	False Omission Rate <input type="text"/>	Negative Predictive Value <input type="text"/>
Accuracy 89%		True Positive Rate 85%	False Positive Rate 11%	Please fill in the missing numbers.	
		False Negative Rate 15%	True Negative Rate 89%		

Predictive Metrics Quiz



		Ground Truth			
TOTAL POPULATION 1000		Condition Positive 65	Condition Negative 935	Prevalence 7%	
Prediction	Prediction Outcome Positive 155	True Positive 55	False Positive 100	Positive Predictive Value 35%	False Discovery Rate 65%
	Prediction Outcome Negative 845	False Negative 10	True Negative 835	False Omission Rate 1%	Negative Predictive Value 99%
Accuracy 89%		True Positive Rate 85%	False Positive Rate 11%	Please fill in the missing numbers.	
		False Negative Rate 15%	True Negative Rate 89%		

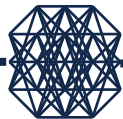
F₁ Score



		Ground Truth			
		TOTAL POPULATION	Condition Positive	Condition Negative	Prevalence = $\frac{\text{Condition Positive}}{\text{Total population}}$
Prediction	Prediction Outcome Positive	True Positive	False Positive (Type I error)	Positive Predictive Value = $\frac{\text{True Positive}}{\text{Prediction outcome positive}}$	False Discovery Rate = $\frac{\text{False Positive}}{\text{Prediction outcome positive}}$
	Prediction Outcome Negative	False Negative (Type II error)	True Negative	False Omission Rate = $\frac{\text{False negative}}{\text{Prediction outcome negative}}$	Negative Predictive Value = $\frac{\text{True negative}}{\text{Prediction outcome negative}}$
Accuracy = $\frac{\text{True positive} + \text{True negative}}{\text{Total population}}$		True Positive Rate = $\frac{\text{True positive}}{\text{Condition positive}}$	False Positive Rate = $\frac{\text{False Positive}}{\text{Condition negative}}$		
		False Negative Rate = $\frac{\text{False negative}}{\text{Condition positive}}$	True Negative Rate = $\frac{\text{True negative}}{\text{Condition negative}}$		

$$F_1 = 2 \times \frac{\text{PPV} \times \text{TPR}}{\text{PPV} + \text{TPR}}$$

F₁ Quiz



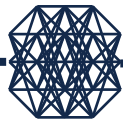
		Ground Truth			
TOTAL POPULATION 1000		Condition Positive 65	Condition Negative 935	Prevalence 7%	
Prediction	Prediction Outcome Positive 155	True Positive 55	False Positive 100	Positive Predictive Value 35%	False Discovery Rate 65%
	Prediction Outcome Negative 845	False Negative 10	True Negative 835	False Omission Rate 1%	Negative Predictive Value 99%
Accuracy 89%		True Positive Rate 85%	False Positive Rate 11%	Please calculate the F₁ score. <input type="text"/>	
		False Negative Rate 15%	True Negative Rate 89%		

F₁ QUIZ



		Ground Truth			
		TOTAL POPULATION 1000	Condition Positive 65	Condition Negative 935	Prevalence 7%
Prediction	Prediction Outcome Positive 155	True Positive 55	False Positive 100	Positive Predictive Value 35%	False Discovery Rate 65%
	Prediction Outcome Negative 845	False Negative 10	True Negative 835	False Omission Rate 1%	Negative Predictive Value 99%
Accuracy 89%		True Positive Rate 85%	False Positive Rate 11%	Please calculate the F₁ score . <div>≈0.5</div>	
		False Negative Rate 15%	True Negative Rate 89%		

Classifier Quiz



Which of these is the best classifier?

☐ **A**

TP=63	FP=28	91
FN=37	TN=72	109
100	100	200

PPV = 0.69
 F_1 = 0.66
Accuracy = 0.68

☐ **B**

TP=77	FP=77	154
FN=23	TN=23	46
100	100	200

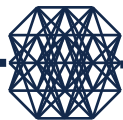
PPV = 0.50
 F_1 = 0.61
Accuracy = 0.50

☒ **C**

TP=76	FP=12	88
FN=24	TN=88	112
100	100	200

PPV = 0.86
 F_1 = 0.81
Accuracy = 0.82

Classifier Quiz 2



Which of these is the best classifier?

☐ **A**

TP=63	FP=28	91
FN=37	TN=72	109
100	100	200

PPV = 0.69
 F_1 = 0.66
ACC = 0.68

☐ **B**

TP=77	FP=77	154
FN=23	TN=23	46
100	100	200

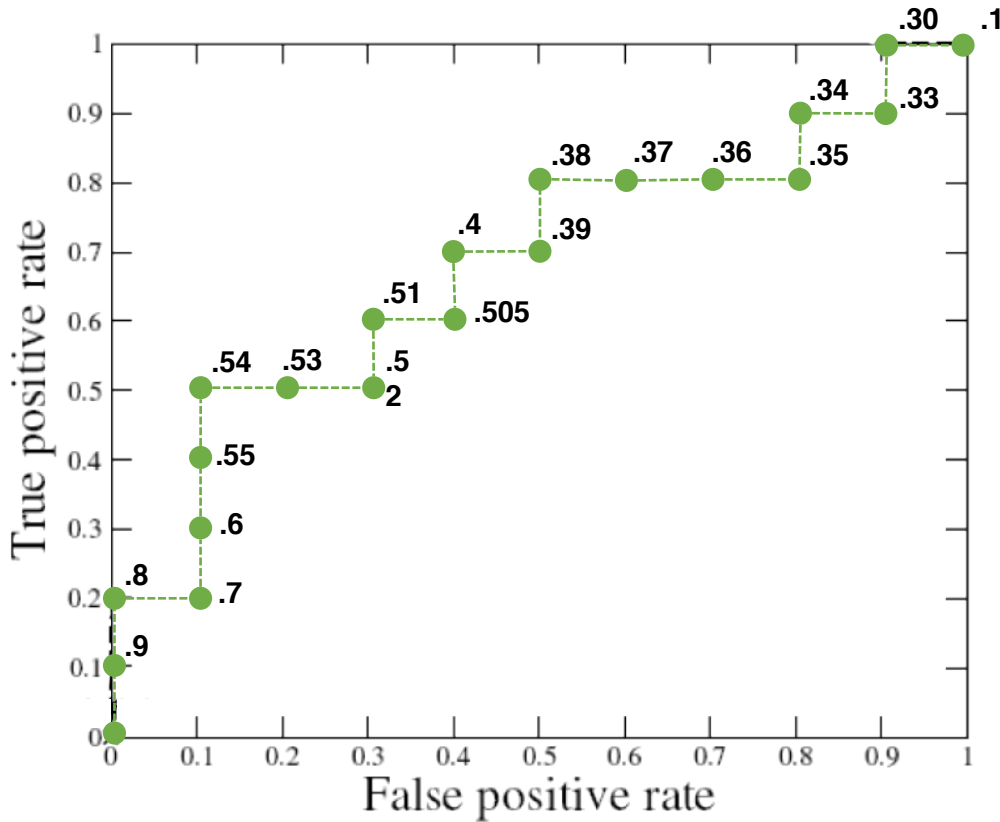
PPV = 0.50
 F_1 = 0.61
ACC = 0.50

☒ **C**

TP=24	FP=88	112
FN=76	TN=12	88
100	100	200

PPV = 0.21 → 0.86
 F_1 = 0.22 → 0.81
ACC = 0.18 → 0.82

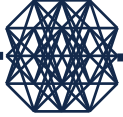
Receiver Operating Characteristic (ROC)



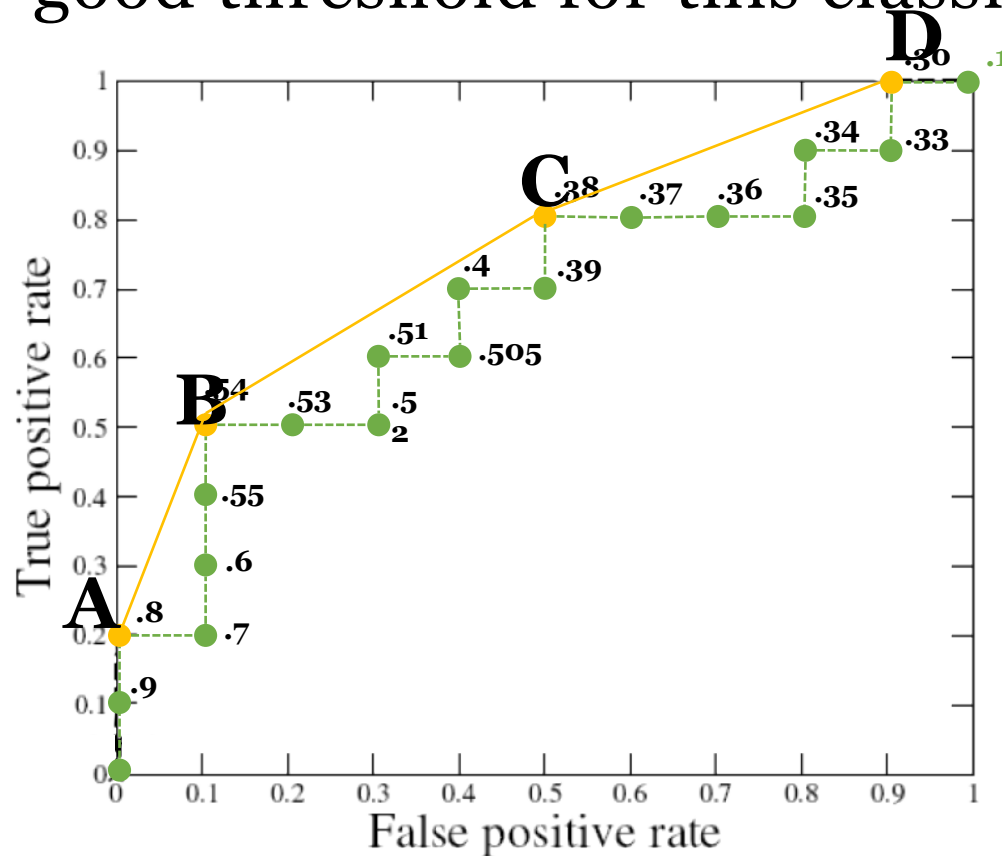
#p = 10, #n=10

Inst#	Class	Score
1	p	.9
2	p	.8
3	n	.7
4	p	.6
5	p	.55
6	p	.54
7	n	.53
8	n	.52
9	p	.51
10	n	.505
11	p	.4
12	n	.39
13	p	.38
14	p	.37
15	n	.36
16	n	.35
17	p	.34
18	n	.33
19	p	.30
20	n	.1

Classification Metric: Roc Quiz



Which of the following would be a good threshold for this classifier?



- ☒ **A**
- ☒ **B**
- ☒ **C**
- ☒ **D**

Inst#	Class	Score
1	p	.9
2	p	.8
3	n	.7
4	p	.6
5	p	.55
6	p	.54
7	n	.53
8	n	.52
9	p	.51
10	n	.505
11	p	.4
12	n	.39
13	p	.38
14	p	.37
15	n	.36
16	n	.35
17	p	.34
18	n	.33
19	p	.30
20	n	.1

Regression Metrics: MAE, MSE

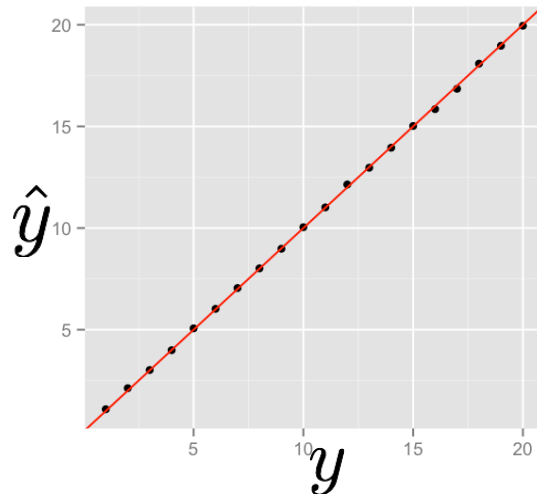


Mean Absolute Error (MAE)

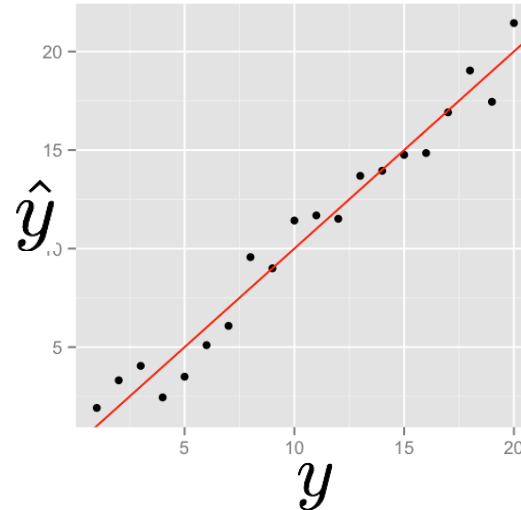
$$MAE = \frac{1}{n} \sum_i |y_i - \hat{y}_i|$$

Mean Squared Error (MSE)

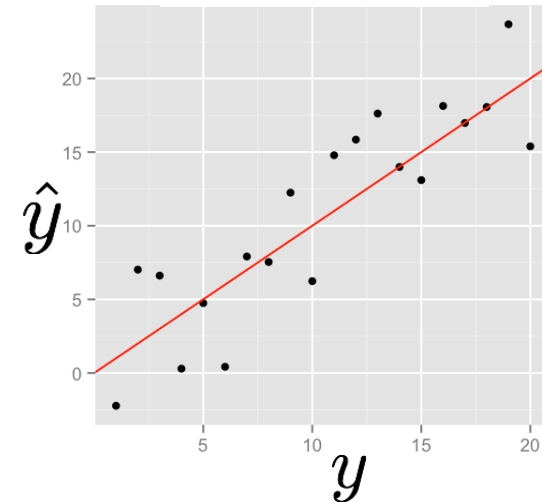
$$MSE = \frac{1}{n} \sum_i (y_i - \hat{y}_i)^2$$



MAE = 0.0837
MSE = 0.0129



MAE = 0.7804
MSE = 1.1883



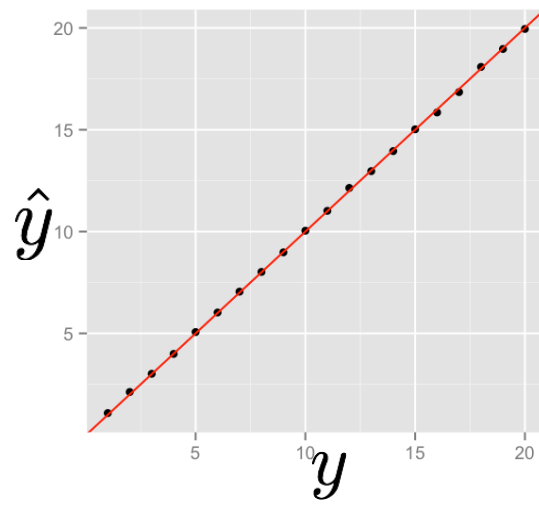
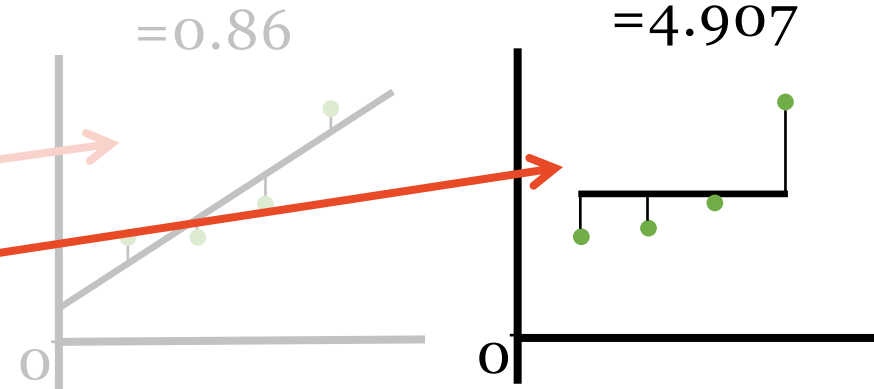
MAE = 3.4328
MSE = 18.6435

Regression Metrics: R^2

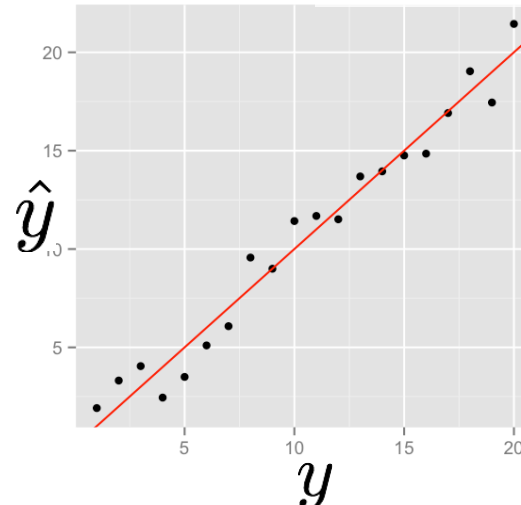


Coefficient of determination R^2

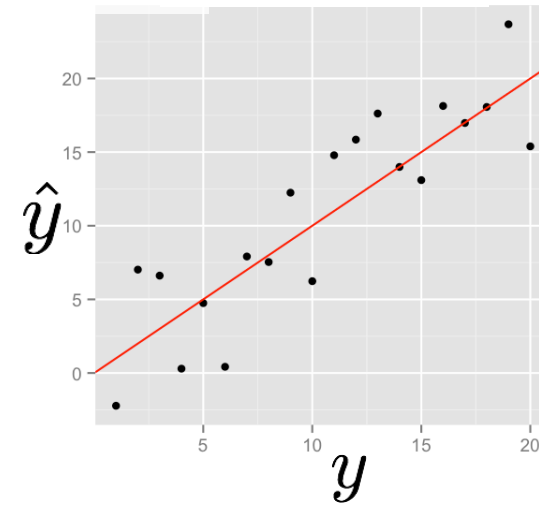
$$R^2 = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$$



$R^2 = 0.9997$

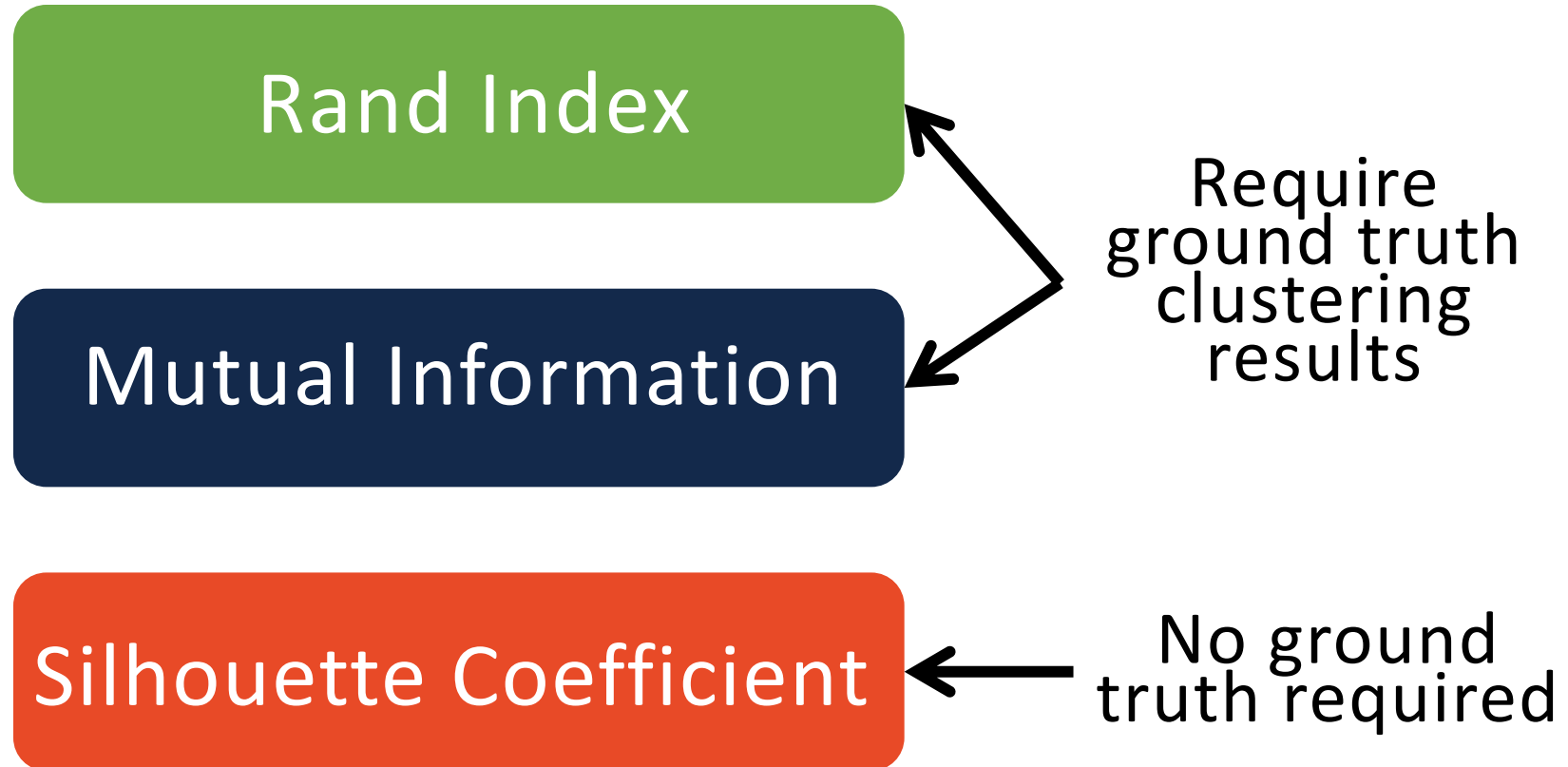


$R^2 = 0.7803$

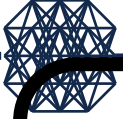


$R^2 = 0.7404$

Clustering Evaluation Metrics



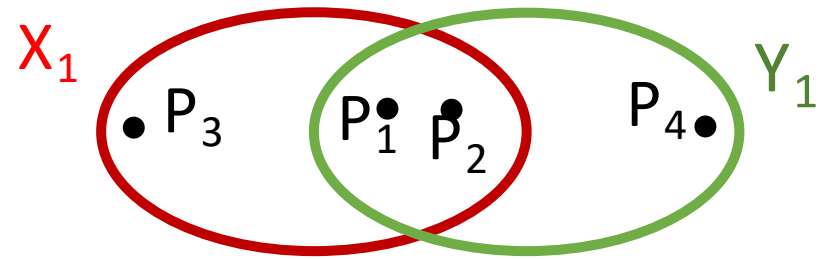
Rand Index (RI)



n data points

X: clustering assignments

Y: ground truth



a: # of pairs that belong to same cluster in X and Y

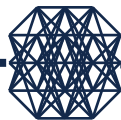
b: # of pairs that belong to different clusters in X and Y

$$RI = \frac{a + b}{\# \text{ of pairs}} \leftarrow \frac{n(n-1)}{2}$$

RI = 0 bad clustering 👎

RI = 1 perfect clustering 👍

Mutual Information



$X = \{x_1, x_2, \dots, x_k\}$ clustering assignments

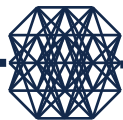
$Y = \{y_1, y_2, \dots, y_r\}$ ground truth

Entropy

$$H(X) = \sum_{x \in X} p(x) \log p(x)$$

deterministic random
[0, 1]

Mutual Information



$X = \{x_1, x_2, \dots, x_k\}$ clustering assignments

$Y = \{y_1, y_2, \dots, y_r\}$ ground truth

deterministic random

Entropy $H(X) = \sum_{x \in X} p(x) \log p(x)$ $[0, 1]$

$$MI(X, Y) = \sum_{x \in X} \sum_{y \in Y} p(x, y) \log \frac{p(x, y)}{p(x)p(y)}$$

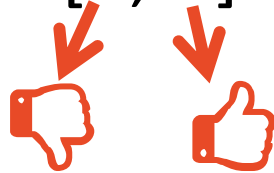
$$\text{Normalized_MI}(X, Y) = \frac{MI(X, Y)}{\sqrt{H(X)H(Y)}}$$

Summary Of Rand Index and Mutual Information



PROS

- Bounded range $[0, 1]$



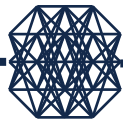
- No assumption on cluster shapes



CONS

- Require ground truth

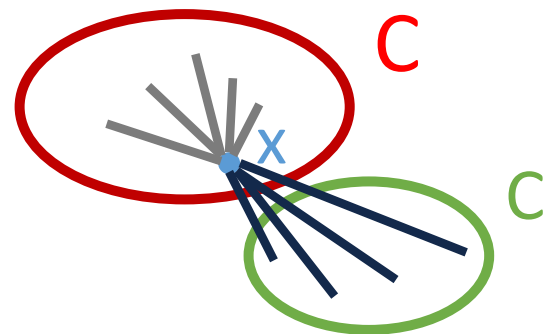
Silhouette Coefficient



x : data point

C : cluster containing x

C' : next nearest cluster to x



$$a = \frac{1}{|C|} \sum_{y \in C} \|x - y\|$$

$$b = \frac{1}{|C'|} \sum_{z \in C'} \|x - z\|$$

$$s(x) = \frac{b - a}{\max(a, b)}$$

Silhouette Coefficient



PROS

- Bounded between -1 and 1



Bad clustering
assignment



Good clustering
assignment



CONS

- Assume spherical clusters