3. Machine Learning Basics

Prof. Jimeng Sun

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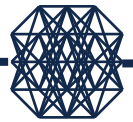
Evaluation metrics



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

Performance Metrics: Classification

		Ground Truth	
	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

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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

Prediction	Prediction Outcome Positive
	Prediction Outcome Negative

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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

Ground Truth	
Condition Positive	Condition Negative

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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

True 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

False Positive
(Type I error)

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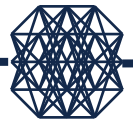
Performance Metrics: Classification



		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

False Negative
(Type II error)

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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

True 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

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Confusion Matrix Quiz

		Ground Truth	
	TOTAL POPULATION	Condition Positive	Condition Negative
			935
Prediction	Prediction Outcome Positive 155	True Positive	False Positive 100
	Prediction Outcome Negative	False Negative 10	True Negative

Please fill in the missing numbers.

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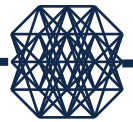
Confusion Matrix Quiz



		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**

Please fill in the missing numbers.

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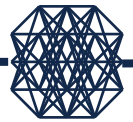
Performance Metrics: Classification



		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 = $\frac{\text{True negative}}{\text{Condition negative}}$

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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 = $\frac{\text{True negative}}{\text{Condition negative}}$

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

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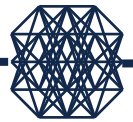
PERFORMANCE METRICS: CLASSIFICATION



		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 = $\frac{\text{True negative}}{\text{Condition negative}}$

False Negative Rate

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

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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 = $\frac{\text{True negative}}{\text{Condition negative}}$

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

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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 = $\frac{\text{True negative}}{\text{Condition negative}}$

True Negative Rate (Specificity) = $\frac{\text{True negative}}{\text{Condition negative}}$

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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	False Positive Rate
		False Negative Rate	True Negative Rate

Please fill in the missing numbers.

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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.

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

Prevalence $= \frac{\text{Condition Positive}}{\text{Total population}}$

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

Positive Predictive Value (Precision)

$$= \frac{\text{True Positive}}{\text{Test outcome positive}}$$

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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 $= \frac{\text{True Positive}}{\text{Prediction outcome positive}}$
	Prediction Outcome Negative	False Negative (Type II error)	True Negative	False Omission Rate $= \frac{\text{False negative}}{\text{Prediction outcome negative}}$
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 $= \frac{\text{True negative}}{\text{Condition negative}}$	

False Discovery Rate $= \frac{\text{False Positive}}{\text{Prediction outcome positive}}$

False Discovery Rate $= \frac{\text{False Positive}}{\text{Prediction outcome positive}}$

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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 $= \frac{\text{True Positive}}{\text{Prediction outcome positive}}$
	Prediction Outcome Negative	False Negative (Type II error)	True Negative	False Omission Rate $= \frac{\text{False negative}}{\text{Prediction outcome negative}}$
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 $= \frac{\text{True negative}}{\text{Condition negative}}$	

		False Discovery Rate $= \frac{\text{False Positive}}{\text{Prediction outcome positive}}$
		Negative Predictive Value $= \frac{\text{True negative}}{\text{Prediction outcome negative}}$

Negative Predictive Value $= \frac{\text{True negative}}{\text{Prediction outcome negative}}$

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

False Omission Rate $= \frac{\text{False negative}}{\text{Prediction outcome negative}}$

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Predictive Metrics Quiz

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

Please fill in the missing numbers.

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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%		
		False Negative Rate 15%	True Negative Rate 89%		

Please fill in the missing numbers.

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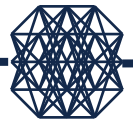
F_1 Score



		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 $= \frac{\text{True negative}}{\text{Condition negative}}$	

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

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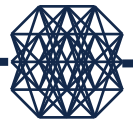
F_1 Quiz



		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%		
		False Negative Rate 15%	True Negative Rate 89%		

Please calculate the F_1 score.

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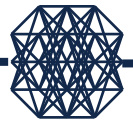
F_1 QUIZ



		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%		
		False Negative Rate 15%	True Negative Rate 89%		

Please calculate the F_1 score.

≈0.5

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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

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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

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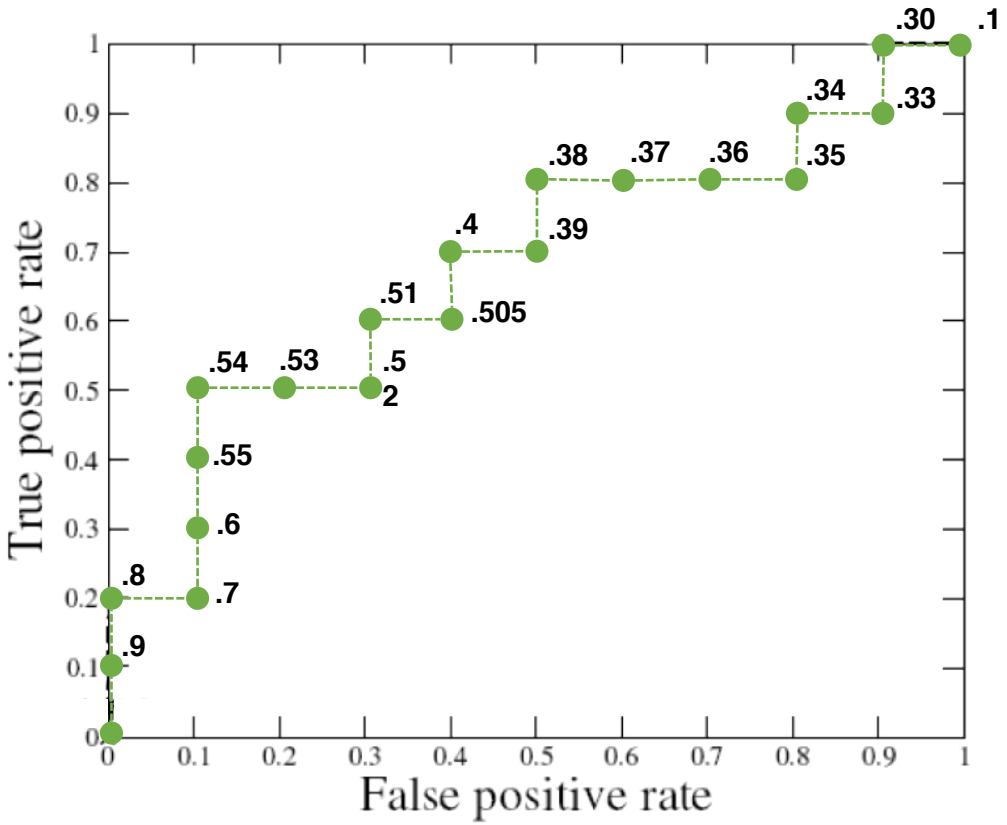
Receiver Operating Characteristic (ROC)



#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

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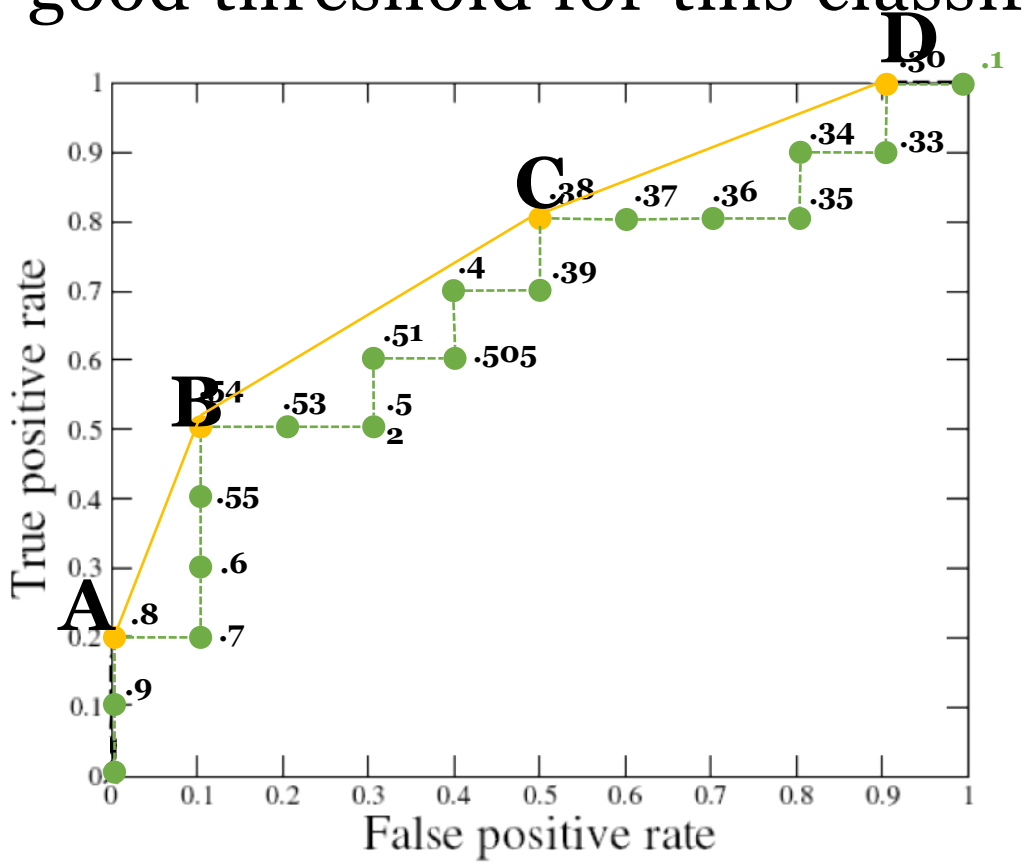
Classification Metric: Roc Quiz

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

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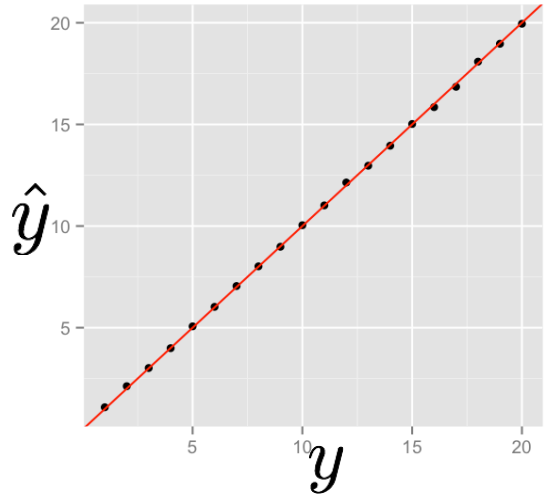
Regression Metrics: MAE, MSE

Mean Absolute Error (MAE)

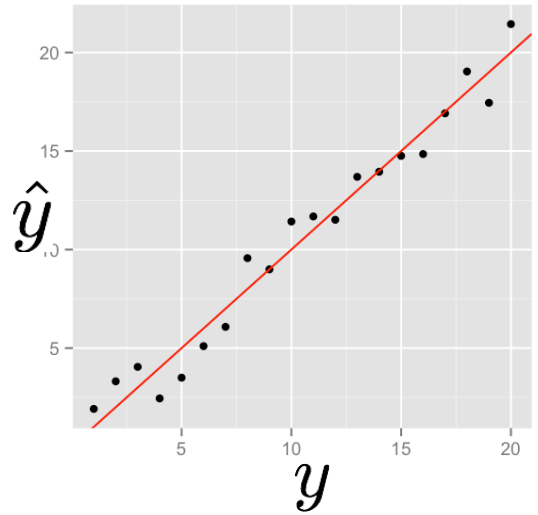
$$MAE = \frac{1}{n}\sum_i |y_i - \hat{y}_i|$$

Mean Squared Error (MSE)

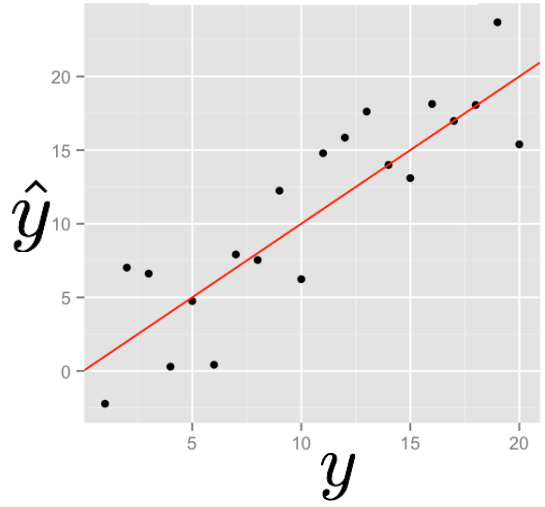
$$MSE = \frac{1}{n}\sum_i (y_i - \hat{y}_i)^2$$



MAE = 0.0837
MSE = 0.0129



MAE = 0.7804
MSE = 1.1883



MAE = 3.4328
MSE = 18.6435

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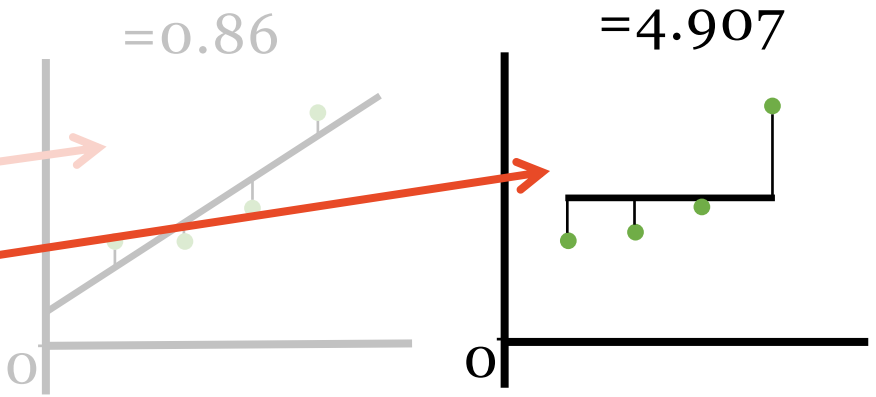
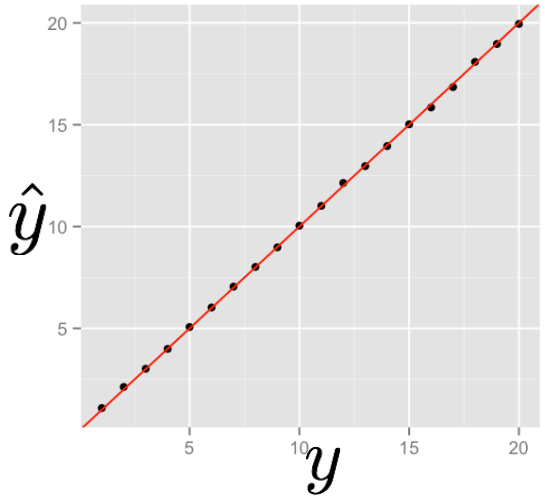
Regression Metrics: R²

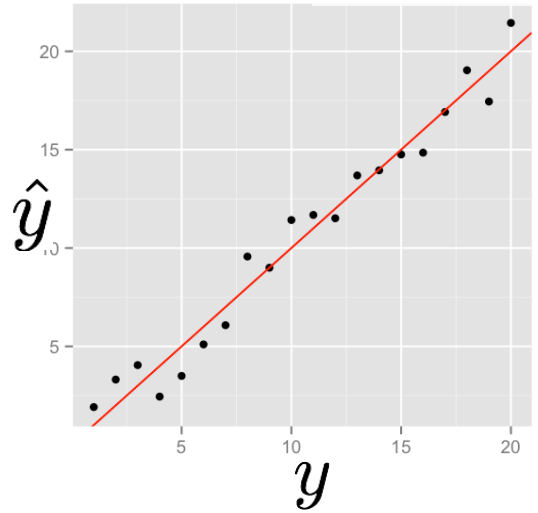
Coefficient of determination R²

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

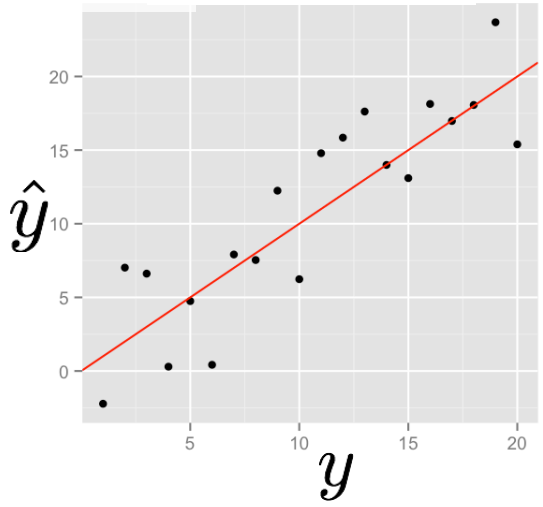




R² =0.9997



R² =0.7803



R² =0.7404

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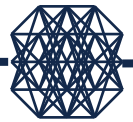
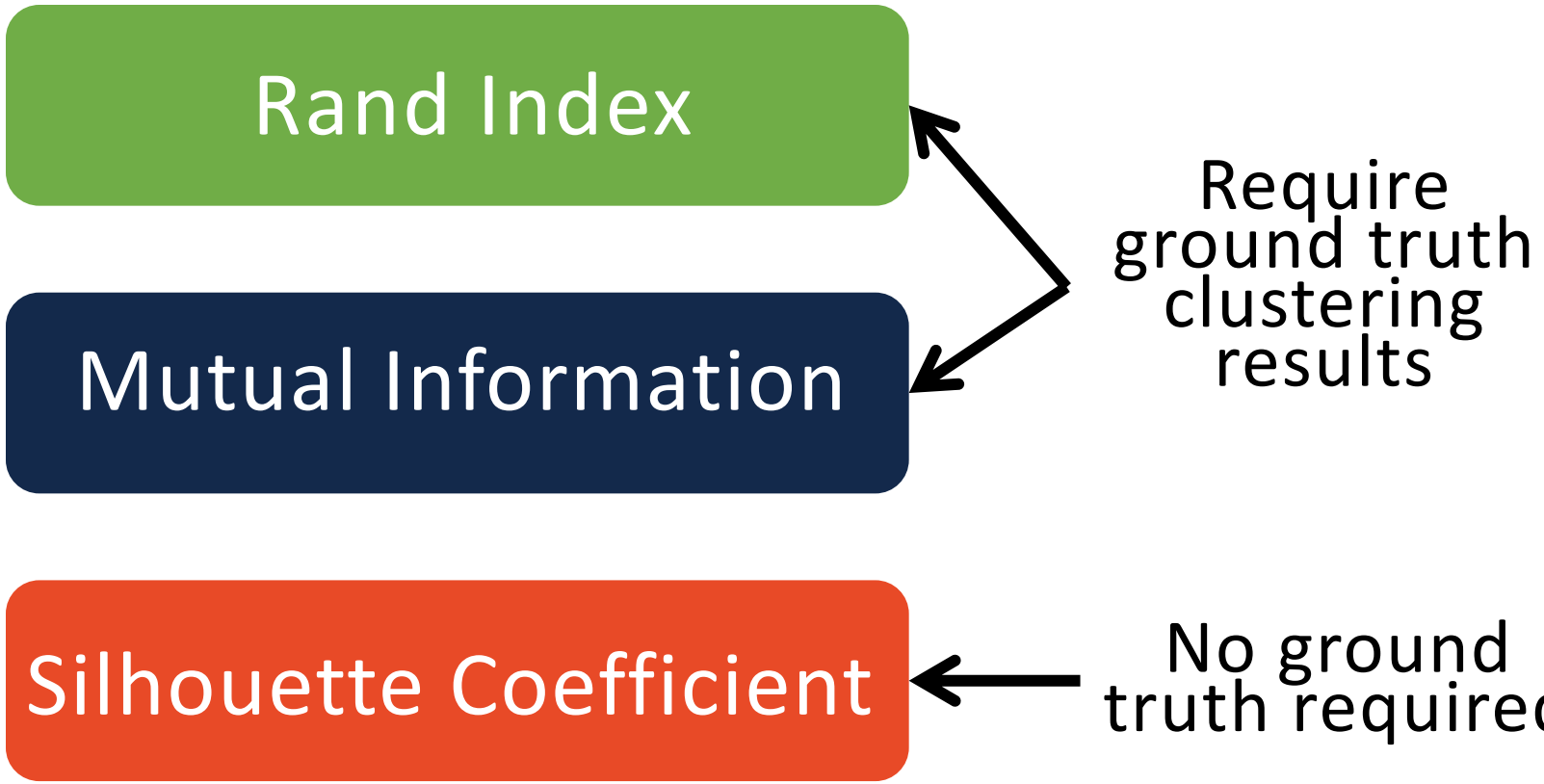
Clustering Evaluation Metrics





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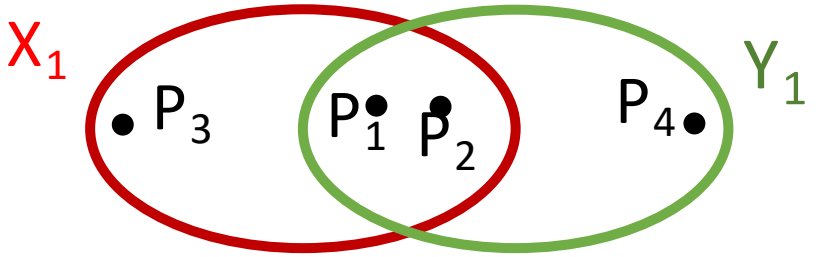
Rand Index (RI)

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

$$\text{RI} = \frac{a+b}{\#\ of\ pairs}$$

$\#\ of\ pairs = \frac{n(n-1)}{2}$

RI = 0 bad clustering

RI = 1 perfect clustering

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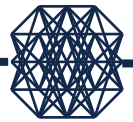
Mutual Information



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

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

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

deterministic random

$[0, 1]$

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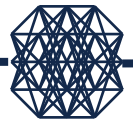
Mutual Information



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

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deterministic random

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

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

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

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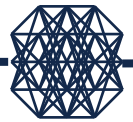
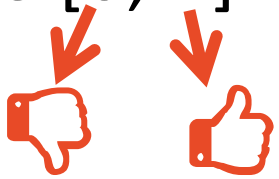
Summary Of Rand Index and Mutual Information



PROS

- Bounded range [0, 1]



- No assumption on cluster shapes

CONS

- Require ground truth

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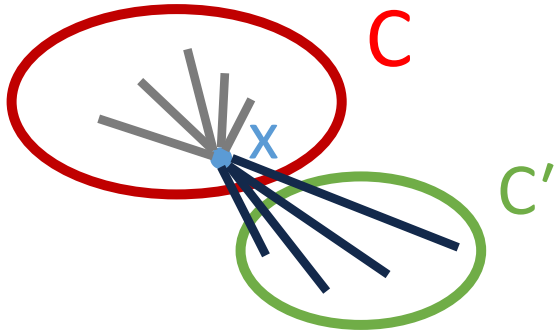
Silhouette Coefficient

x: data point

C: cluster containing x

C′: next nearest cluster to x



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

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

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

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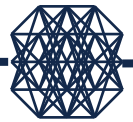
Silhouette Coefficient



PROS

- Bounded between -1 and 1

Bad clustering assignment

Good clustering assignment

CONS

- Assume spherical clusters

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