

# Instituto de Computação UNIVERSIDADE ESTADUAL DE CAMPINAS



# Capacitação profissional em tecnologias de Inteligência Artificial

# **Machine Learning Overview**

**Prof. Edson Borin** 

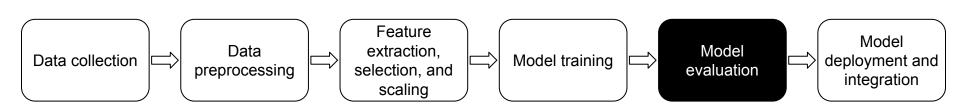
https://www.ic.unicamp.br/~edson
Institute of Computing - UNICAMP



### **ML Process**



# Model evaluation (II) Performance measures







# Performance measures: regression tasks

Usually distance between  $h_{\theta}(x^{(i)})$  and  $y^{(i)}$ 

RMSE: Root Mean Square Error

RMSE(X,h<sub>\theta</sub>) = 
$$\sqrt{\frac{1}{m}} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

MAE: Mean Absolute Error

MAE(X,
$$h_{\theta}$$
) =  $\frac{1}{m} \sum_{i=1}^{m} |h_{\theta}(x^{(i)}) - y^{(i)}|$ 





# Performance measures: regression tasks

Usually distance between  $h_{\theta}(x^{(i)})$  and  $y^{(i)}$ 

MSE: Mean Square Error

RMSE = 
$$\sqrt{MSE}$$

MSE(X,h<sub>\theta</sub>) = 
$$\frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$





# Performance measures: regression tasks

Usually distance between  $h_{\rho}(x^{(i)})$  and  $y^{(i)}$ 

• R<sup>2</sup>: Coefficient of determination (a.k.a. "R squared")

$$\overline{y} = \frac{1}{m} \sum_{i=1}^{m} y^{(i)}$$

$$SS_{res} \qquad \sum_{i=1}^{m} (y^{(i)})$$

$$R^{2}(X,h_{\theta}) = 1 - \frac{SS_{res}}{SS_{tot}} = 1 - \frac{\sum_{i=1}^{m} (y^{(i)} - h_{\theta}(x^{(i)}))}{\sum_{i=1}^{m} (y^{(i)} - \overline{y})^{2}}$$





Ranges from -∞ to 1 and indicates gression tasks how well the model fits data.

distance between  $h_{\theta}(x^{(i)})$  and  $y^{(i)}$ 

• R<sup>2</sup>: Coefficient of determination (a.k.a. "R squared")

$$\overline{y} = \frac{1}{m} \sum_{i=1}^{m} y^{(i)}$$

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#### Performance measures: classification tasks

•  $h_{\theta}(x_1, x_2, ..., x_n) \rightarrow \{1, 2, ..., k\}$ 

Map features to classes

• Distance measures (e.g.,  $h_{\theta}(x^{(i)})$  -  $y^{(i)}$ ) do not reflect well the performance of the classifier





#### Performance measures: classification tasks

•  $h_{\theta}(x_1, x_2, ..., x_n) \rightarrow \{1, 2, ..., k\}$ 

Map features to

- Distance measures (e.g.,  $h_{\theta}(x^{(i)})$   $y^{(i)}$ ) do not reflect well the performance of the classifier
- Ex: for a given sample  $(x^{(i)}, y^{(i)})$ , assume:

$$y^{(i)} = 2$$

$$h_{\theta'}(x^{(i)}) = 3 \Rightarrow h_{\theta'}(x^{(i)}) - y^{(i)} = 3-2 = 1$$

$$\begin{array}{cccc} \circ & h_{\theta'}(x^{(i)}) = 3 & \Rightarrow & h_{\theta'}(x^{(i)}) - y^{(i)} = 3-2 = 1 \\ \circ & h_{\theta''}(x^{(i)}) = 7 & \Rightarrow & h_{\theta''}(x^{(i)}) - y^{(i)} = 7-2 = 5 \end{array}$$





#### Performance measures: classification tasks

•  $h_{\theta}(x_1, x_2, ..., x_n) \rightarrow \{1, 2, ..., k\}$ 

Map features to classes

- Distance measures (e.g.,  $h_{\theta}(x^{(i)})$   $y^{(i)}$ ) do not reflect well the performance of the classifier
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- Confusion matrix
- Accuracy / Error rate
- Precision
- Recall
- F-score





- Confusion matrix: table that shows, for each class, how many of its samples where predicted as each one of the possible classes
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$   $(x_1, x_2, ..., x_n) \to \{$

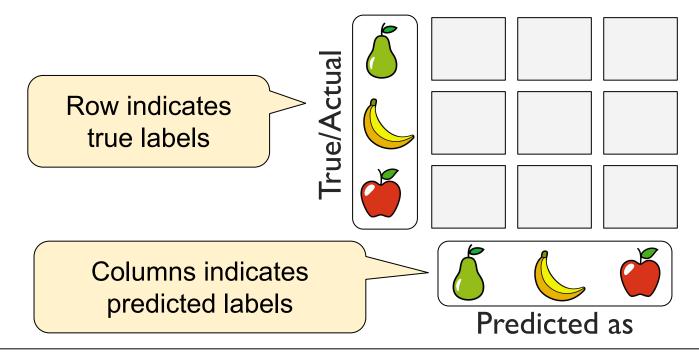








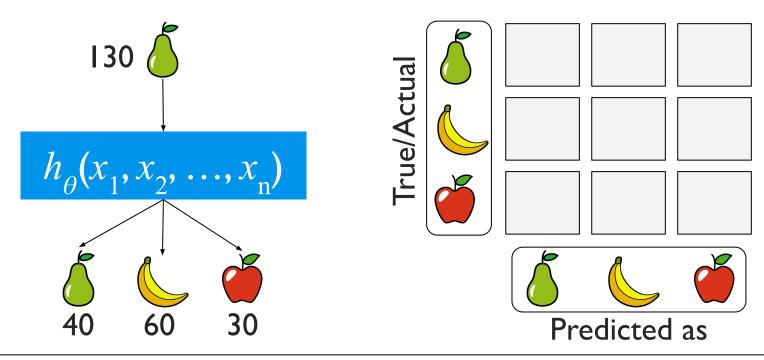
- Confusion matrix: table that shows, for each class, how many of its samples where predicted as each one of the possible classes
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{ (0, (0, 1)) \}$







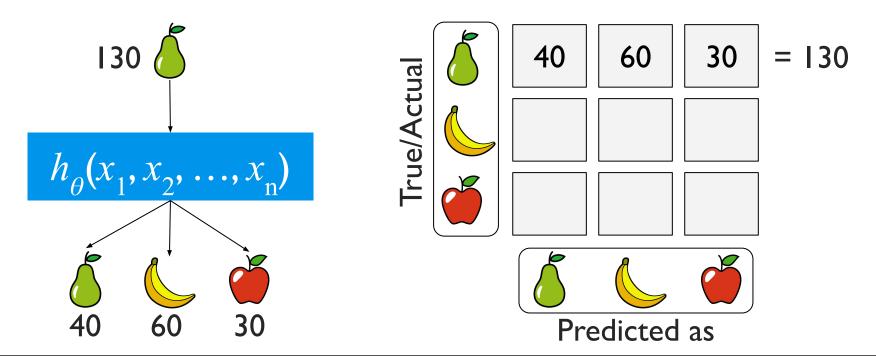
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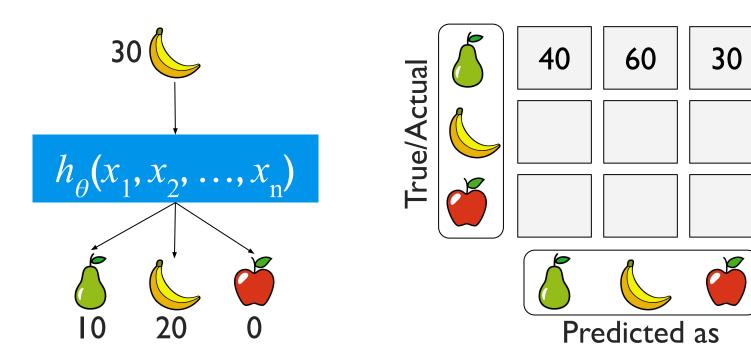
- Confusion matrix: table that shows, for each class, how many of its samples where predicted as each one of the possible classes
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{ b, b \}$







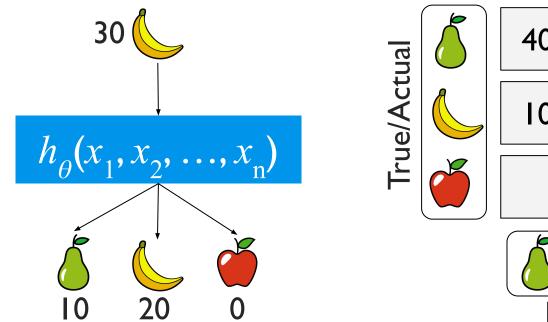
- Confusion matrix: table that shows, for each class, how many of its samples where predicted as each one of the possible classes
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{ (5, (5, 1)) \}$

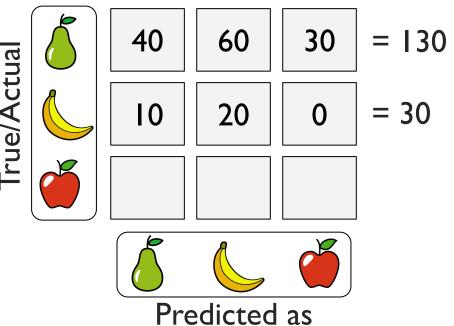






- Confusion matrix: table that shows, for each class, how many of its samples where predicted as each one of the possible classes
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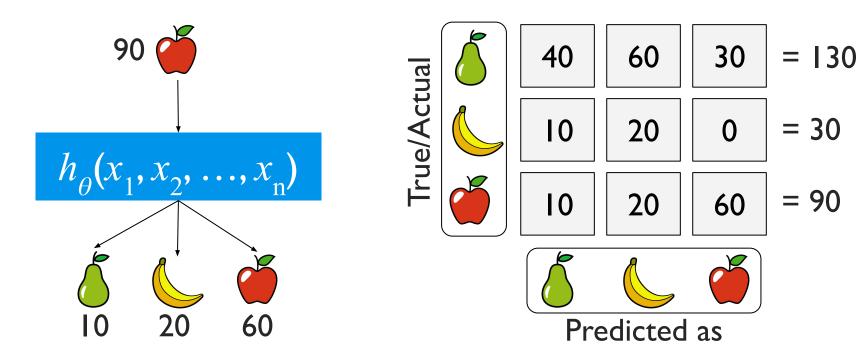








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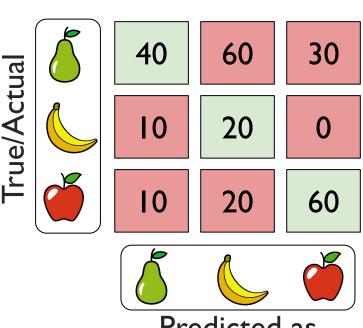


#### Performance measures: classification tasks

- Confusion matrix: table that shows, for each class, how many of its samples where predicted as each one of the possible classes
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$



Incorrect prediction



Predicted as

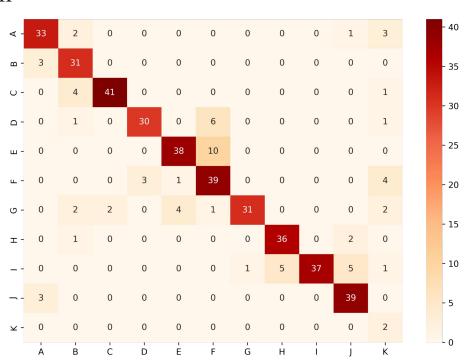




#### Performance measures: classification tasks

- Confusion matrix: table that shows, for each class, how many of its samples where predicted as each one of the possible classes
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{A, B, ..., K\}$

Confusion matrix colored with **Heatmap** 





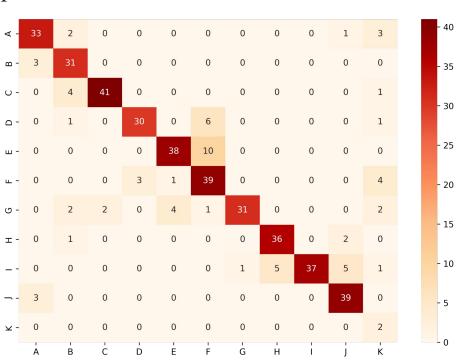


#### Performance measures: classification tasks

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Confusion matrix colored with Heatmap

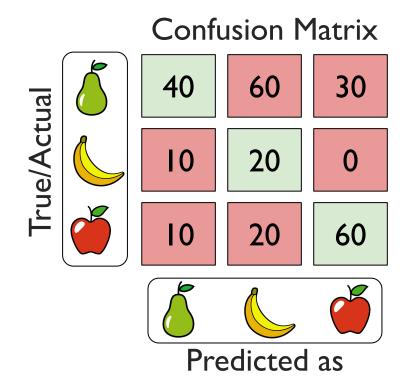
Sometimes is useful to summarize the whole result as a single number (e.g., accuracy)







- Accuracy = all correct predictions / all predictions.
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$   $(x_1, x_2, ..., x_n) \to \{$





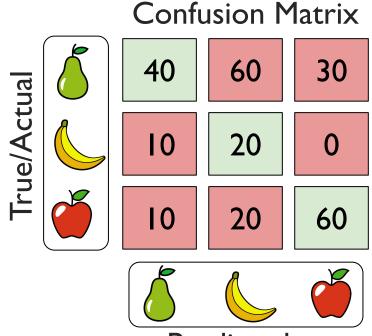


#### Performance measures: classification tasks

- Accuracy = all correct predictions / all predictions.
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$   $(x_1, x_2, ..., x_n) \to \{$

Accuracy = 120/250 = 48%

Summarizes all results





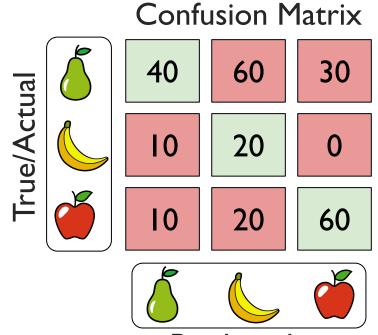


#### Performance measures: classification tasks

- Error rate = all incorrect predictions / all predictions.
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$

Error rate = 130/250 = 52%

error rate = 1 - accuracy



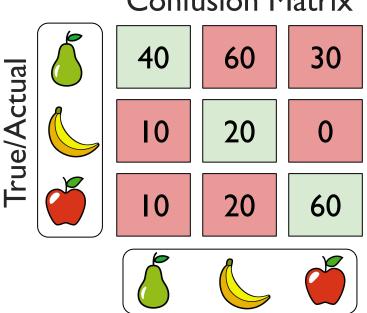




#### Performance measures: classification tasks

<u>Precision</u> = proportion of samples predicted as class X that really belong to class X.

• Example:  $h_{\theta}(x_1, x_2, ..., x_n) \rightarrow \{$  Confusion Matrix



Predicted as





#### Performance measures: classification tasks

 <u>Precision</u> = proportion of samples predicted as class X that really belong to class X.

• Example:  $h_{\theta}(x_1, x_2, ..., x_n) \rightarrow \{$  Confusion Matrix

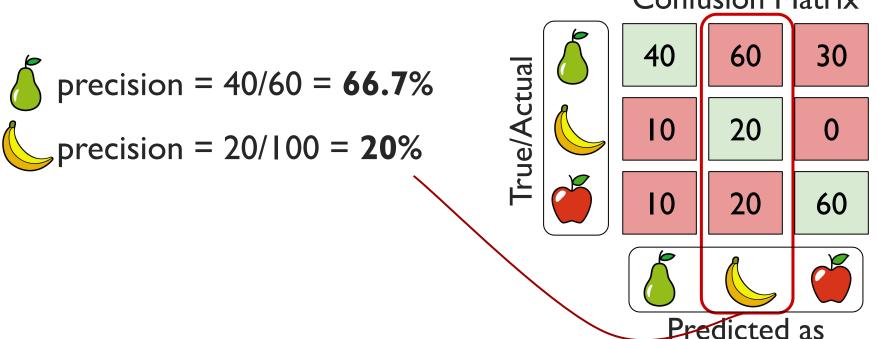
precision = 40/60 = 66.7%

| Variable | Vari





- <u>Precision</u> = proportion of samples predicted as class X that really belong to class X.
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \rightarrow \{$  Confusion Matrix







### Performance measures: classification tasks

- <u>Precision</u> = proportion of samples predicted as class X that really belong to class X.
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{ (0, (0, 1)) \}$ Confusion Matrix

60 30 40 rue/Actua precision = 40/60 = 66.7%20 precision = 20/100 = **20**% 20 60 precision = 60/90 = 66.7%

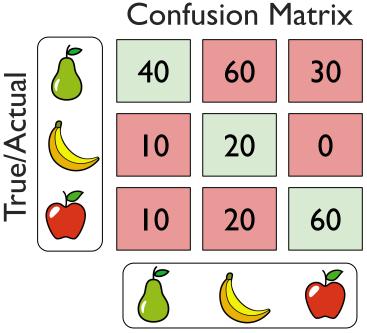




#### Performance measures: classification tasks

- Recall = proportion of class X samples classified correctly
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$   $(x_1, x_2, ..., x_n) \to \{$



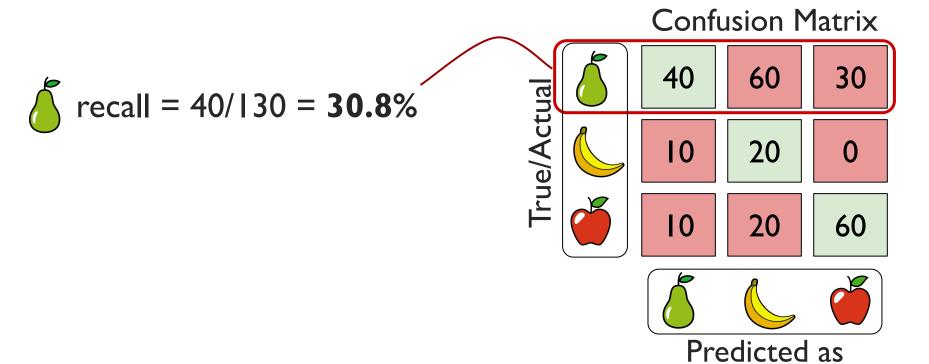


Predicted as





- Recall = proportion of class X samples classified correctly
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$   $(x_1, x_2, ..., x_n) \to \{$



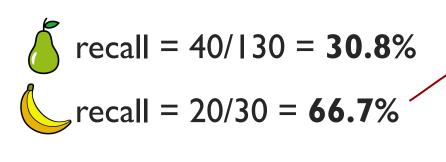


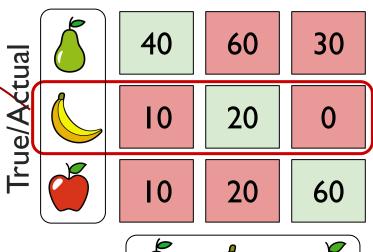


#### Performance measures: classification tasks

- Recall = proportion of class X samples classified correctly
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$   $(x_1, x_2, ..., x_n) \to \{$

#### Confusion Matrix







Predicted as

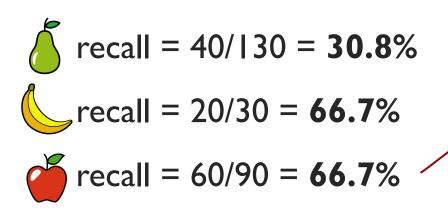


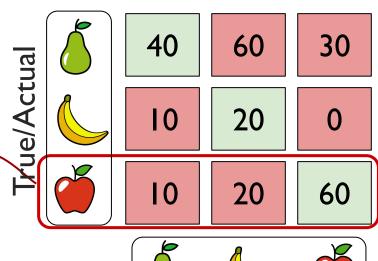


# Performance measures: classification tasks

- Recall = proportion of class X samples classified correctly
- Example:  $h_{\theta}(x_1, x_2, ..., x_n) \to \{$   $(x_1, x_2, ..., x_n) \to \{$

#### Confusion Matrix



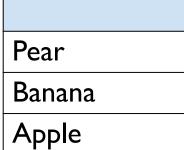






- Summarizing Recall and Precision
  - $\circ$  F<sub>1</sub>-score = (2 × precision × recall) / (precision + recall)
  - macro vs weighted average

	5	
	)	
1		



Precision	Recall
66.7%	30.8%
20%	66.7%
66.7%	66.7%





# Performance measures: classification

Precision and recall Harmonic mean

- Summarizing Recall and Precision
  - $\circ$  F<sub>1</sub>-score = (2 × precision × recall) / (precision + recall)
  - macro vs weighted average

	Precision	Recall	F <sub>1</sub> -score
Pear	66.7%	30.8%	42.1%
Banana	20%	66.7%	30.8%
Apple	66.7%	66.7%	66.7%





#### Performance measures: classification tasks

- Summarizing Recall and Precision
  - $\circ$  F<sub>1</sub>-score = (2 × precision × recall) / (precision + recall)
  - macro vs weighted average

	Precision	Recall	F <sub>1</sub> -score
Pear	66.7%	30.8%	42.1%
Banana	20%	66.7%	30.8%
Apple	66.7%	66.7%	66.7%
Macro avg	51.1%	54.73	46.5%
Weighted avg	61.1%	48.0%	49.6%
	Banana Apple Macro avg	Pear       66.7%         Banana       20%         Apple       66.7%         Macro avg       51.1%	Pear       66.7%       30.8%         Banana       20%       66.7%         Apple       66.7%       66.7%         Macro avg       51.1%       54.73

Weighted by the number of samples

Accuracy = 120/250 = 48%





Pei

from sklearn import metrics print(metrics.classification\_report(y\_true, y\_pred, digits=3))

	precision	recall f	f1-score	support
Apple	0.667	0.667	0.667	90
Banana	0.200	0.667	0.308	30
Pear	0.667	0.308	0.421	130
accuracy			0.480	250
macro avg	0.511	0.547	0.465	250
weighted avg	0.611	0.480	0.496	250

130 🍊

30 📞

90 🍊

		Precision	Recall	F <sub>1</sub> -score
	Pear	66.7%	30.8%	42.1%
	Banana	20%	66.7%	30.8%
)	Apple	66.7%	66.7%	66.7%
	Macro avg	51.1%	54.73	46.5%
	Weighted avg	61.1%	48.0%	49.6%

scikit learn classification report

Accuracy = 120/250 = 48%





### Performance measures: classification tasks

$$F_{\beta}\text{-score} = \frac{(1+\beta^2) \times \text{precision} \times \text{recall}}{(\beta^2 \times \text{precision}) + \text{recall}}$$

$$F_1$$
-score = 
$$\frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

 $F_1$ -score is a special case of  $F_{\beta}$ -score ( $\beta$ =1)





# Performance measures: **classification tasks** P. N.TP, FP, TN, FN

- On binary classifiers, precision and recall are usually expressed as a function of Positives, Negatives, True Positive (TP), False Positives (FP), True Negative (TN), and False Negatives (FN)
- For a given class X
  - Positives: samples predicted as class X
    - TP (True Positives) samples correctly predicted as X
    - FP (False Positives) samples incorrectly predicted as X
  - Negatives: samples predicted as non-X (other classes)
    - TN (True Negative) samples correctly predicted as non-X
    - FN (False Negative) samples incorrectly predicted as non-X





# Performance measures: **classification tasks** P. N.TP, FP, TN, FN

Ex: Credit card fraud



Fraud



Legitimate transaction

#### Positives: samples predicted as fraud

- TP: correctly predicted as fraud
- FP: incorrectly predicted as fraud

#### Negatives: samples predicted as non-fraud

- TN: correctly predicted as non-fraud (legit)
- FN: incorrectly predicted as non-fraud (legit)





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



Legitimate transaction

# 467 6456

#### Positives: samples predicted as fraud

- TP: correctly predicted as fraud
- FP: incorrectly predicted as fraud

Negatives: samples predicted as non-fraud

- TN: correctly predicted as non-fraud (legit)
- FN: incorrectly predicted as non-fraud (legit)

A	
Pred	icted as

Confusion Matrix

Positives	6923
TP	
FP	
Negatives	
TN	
FN	





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



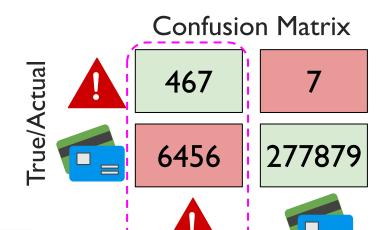
Legitimate transaction

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- TP: correctly predicted as fraud
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Positives	6923
TP	
FP	
Negatives	
TN	
FN	





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



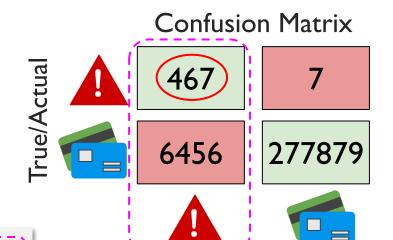
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Positives	6923
TP	467
FP	
Negatives	
TN	
FN	





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



Legitimate transaction

## Positives: samples predicted as fraud

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Confusion Matrix		
Actual	467 <b>TP</b>	7
True//	6456	277879

Positives	6923
TP	467
FP	
Negatives	
TN	
FN	





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



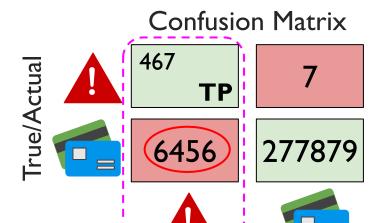
Legitimate transaction

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- (FP:)ncorrectly predicted as fraud

Negatives: samples predicted as non-fraud

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- FN: incorrectly predicted as non-fraud (legit)



Positives	6923
TP	467
FP	6456
Negatives	
TN	
FN	





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



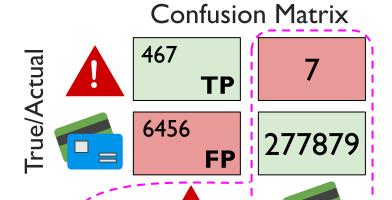
Legitimate transaction

# Positives: samples predicted as fraud

- TP: correctly predicted as fraud
- FP: incorrectly predicted as fraud

# Negatives: samples predicted as non-fraud

- TN: correctly predicted as non-fraud (legit)
- FN: incorrectly predicted as non-fraud (legit)



Positives	6923
TP	467
FP	6456
Negatives	277886
TN	
FN	





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



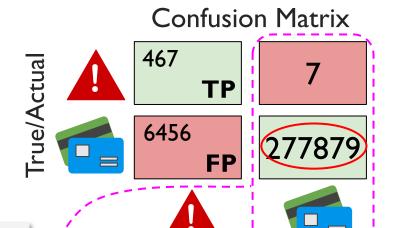
Legitimate transaction

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Positives	6923
TP	467
FP	6456
Negatives	277886
TN	277879
FN	





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



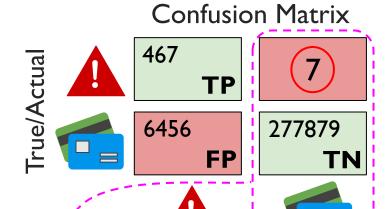
Legitimate transaction

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Positives	6923
TP	467
FP	6456
Negatives	277886
TN	277879
FN	(7)





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



Legitimate transaction

# 467 TP FN 6456 FP TN

#### Positives: samples predicted as fraud

- TP: correctly predicted as fraud
- FP: incorrectly predicted as fraud

#### Negatives: samples predicted as non-fraud

- TN: correctly predicted as non-fraud (legit)
- FN: incorrectly predicted as non-fraud (legit)



Confusion Matrix

Positives	6923
TP	467
FP	6456
Negatives	277886
TN	277879
FN	7





# Performance measures: classification tasks



Ex: Credit card fraud

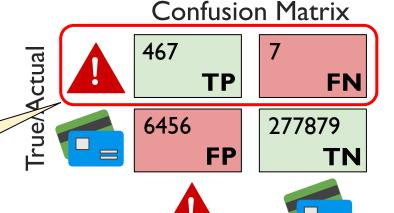


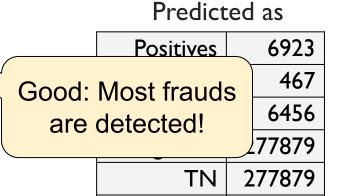
Fraud



Legitimate transaction

$$recall = \frac{1P}{TP+FN} = 98.5\%$$





FN





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



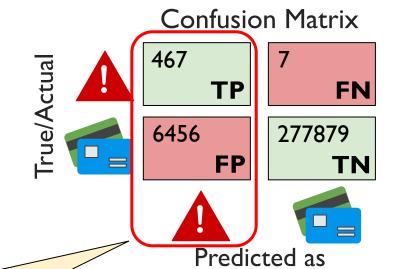
Fraud



Legitimate transaction

$$recall = \frac{TP}{TP+FN} = 98.5\%$$

precision = 
$$\frac{TP}{TP+FP} = \frac{TP}{P} = 6.7\%$$



**Positives** 

TP

Problem: Many legit transactions flagged as fraud!

6923

467





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



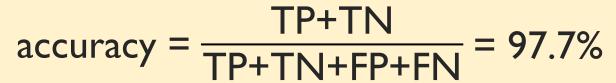
Fraud

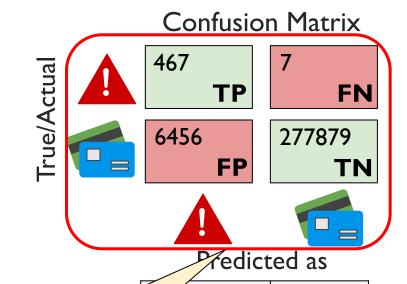


Legitimate transaction

$$recall = \frac{TP}{TP+FN} = 98.5\%$$

precision = 
$$\frac{TP}{TP+FP}$$
 = 6.7%





Positives

11	TO/
FP	6456
Negatives	277879
TN	277879
FN	7

6923





# Performance measures: classification tasks

# <u>P, N, TP, FP, TN, FN</u>

Ex: Credit card fraud



Fraud



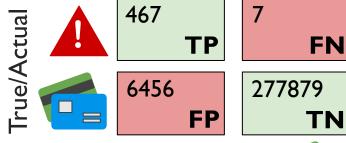
Legitimate transaction

$$recall = \frac{TP}{TP+FN} = 98.5\%$$

precision = 
$$\frac{TP}{TP+FP}$$
 = 6.7%

accuracy = 
$$\frac{TP+TN}{TP+TN+FP+FN} = 97.7\%$$

#### Confusion Matrix



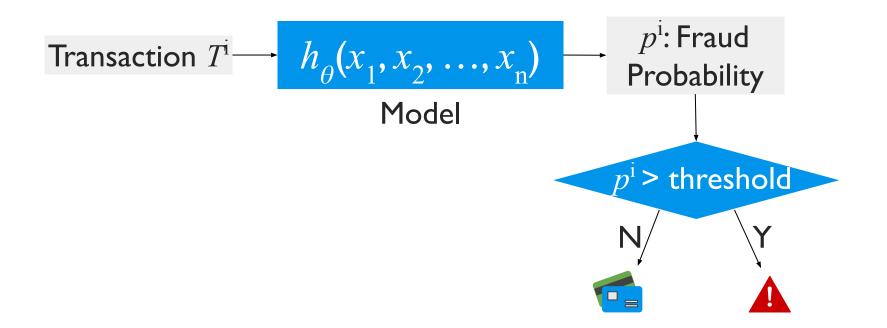


Positives	6923
TP	467
FP	6456
Negatives	277879
TN	277879
FN	7





- Precision/Recall tradeoff
  - Many classifiers can be adjusted to favor precision or recall
  - Ex:Threshold based classifier







# Performance measures: classification tasks

- Precision/Recall tradeoff
  - Many classifiers can be adjusted to favor precision or recall
  - Ex:Threshold based classifier

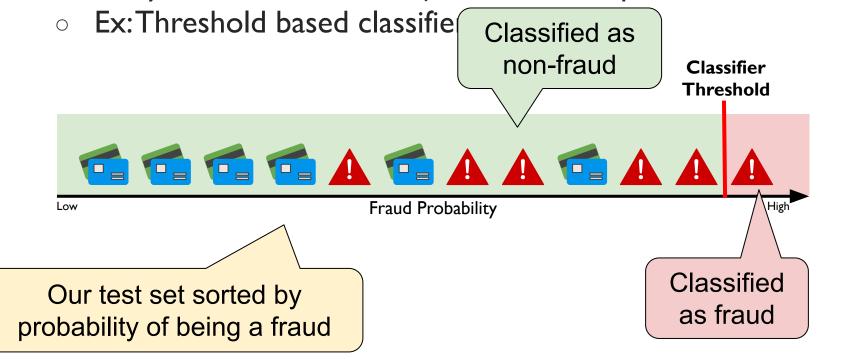


Our test set sorted by probability of being a fraud





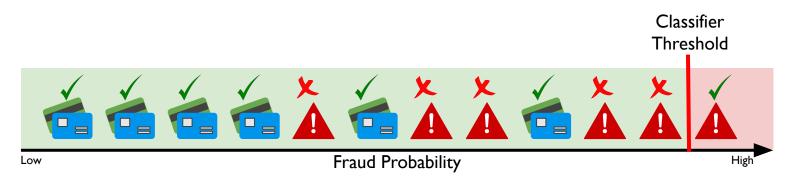
- Precision/Recall tradeoff
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- Precision/Recall tradeoff
  - Many classifiers can be adjusted to favor precision or recall
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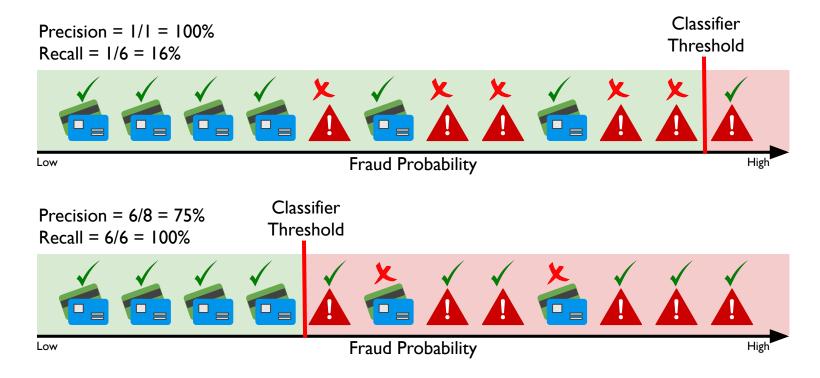
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  - Many classifiers can be adjusted to favor precision or recall
  - Ex:Threshold based classifier





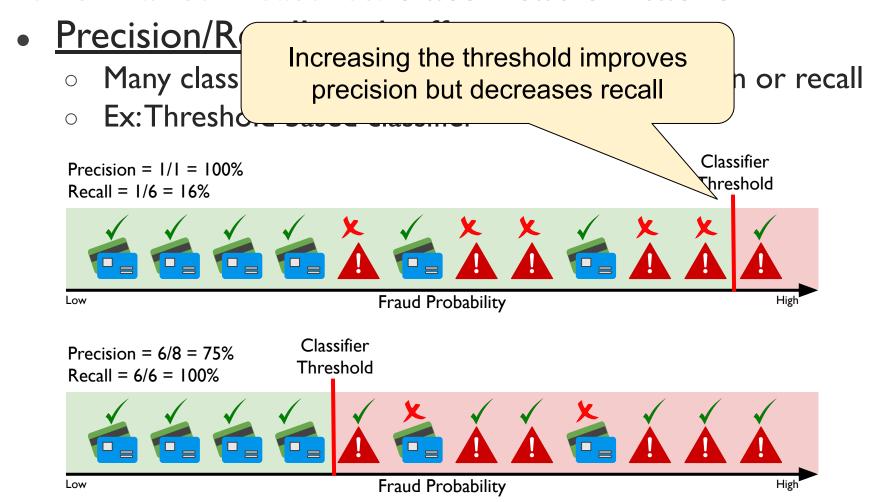


- Precision/Recall tradeoff
  - Many classifiers can be adjusted to favor precision or recall
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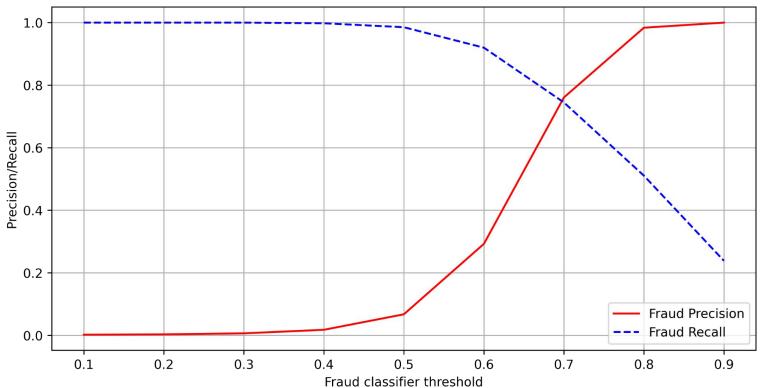








- Precision/Recall tradeoff
  - Many classifiers can be adjusted to favor precision or recall
  - Ex:Threshold based classifier







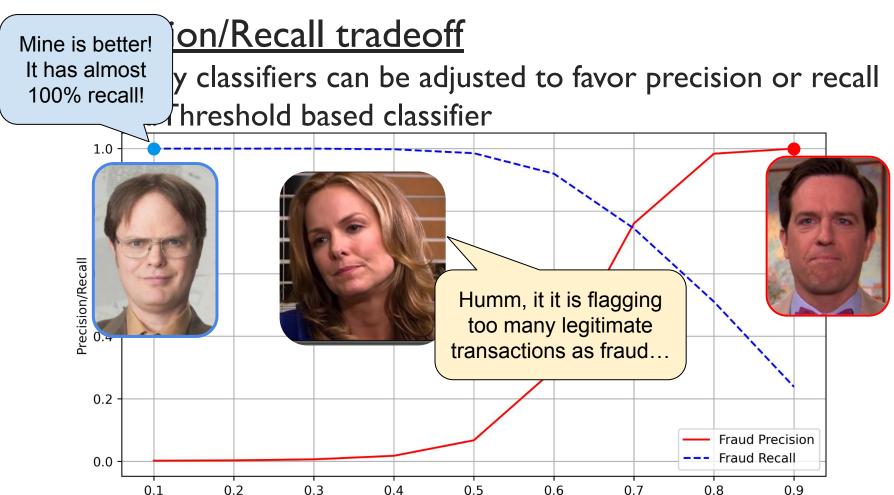
Performance measures: classification tasks My model is Precision/Recall tradeoff great, it has almost 100% Many classifiers can be adjusted to favor preci precision! Ex: Threshold based classifier 1.0 Look, it it is missing too 8.0 many fraudulent transactions Precision/Recall .0 .0 .0 0.2 Fraud Precision Fraud Recall 0.0 0.2 0.3 0.5 0.7 0.1 0.4 0.6 8.0 0.9

Fraud classifier threshold





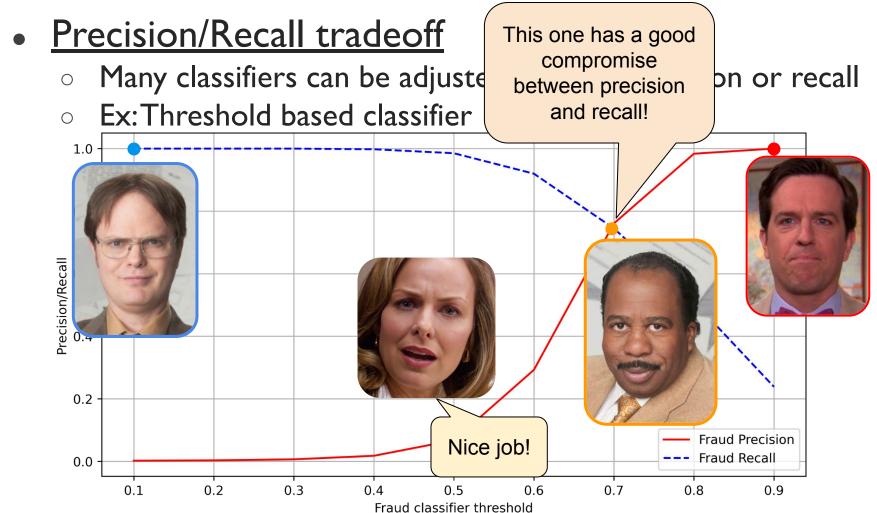
# Performance measures: classification tasks



Fraud classifier threshold



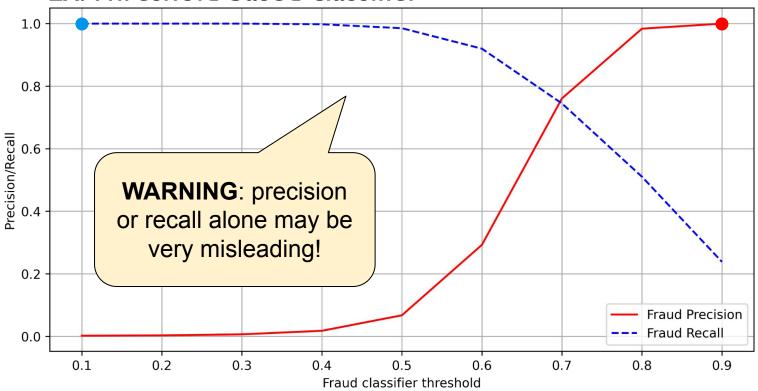








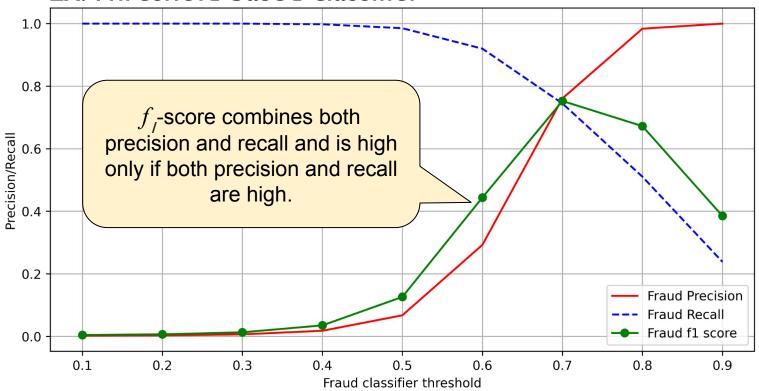
- Precision/Recall tradeoff
  - Many classifiers can be adjusted to favor precision or recall
  - Ex:Threshold based classifier







- Precision/Recall tradeoff
  - Many classifiers can be adjusted to favor precision or recall
  - Ex:Threshold based classifier





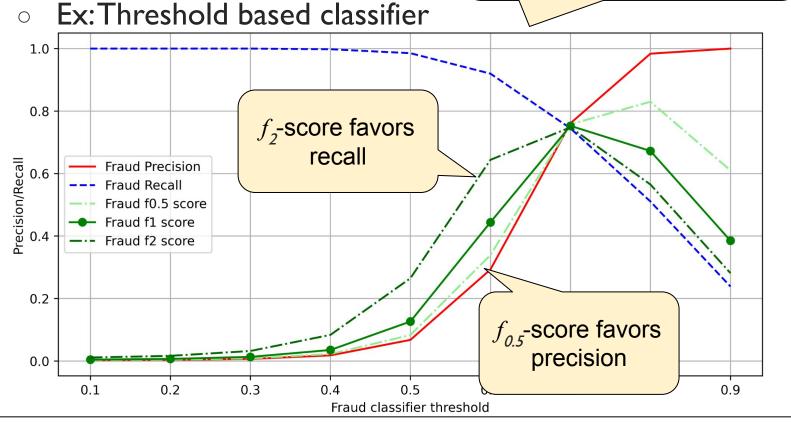


Performance measures: classification tasks

• Precision/Recall tradeoff

Many classifiers can be adjusted

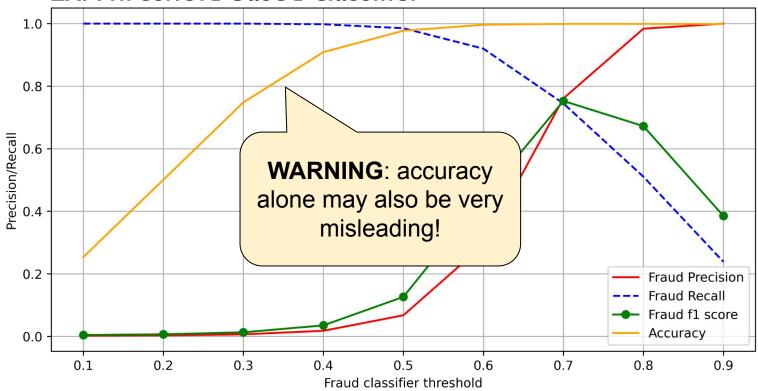
 $f_{\beta}$ -score can be used to assign more importance to precision or recall.





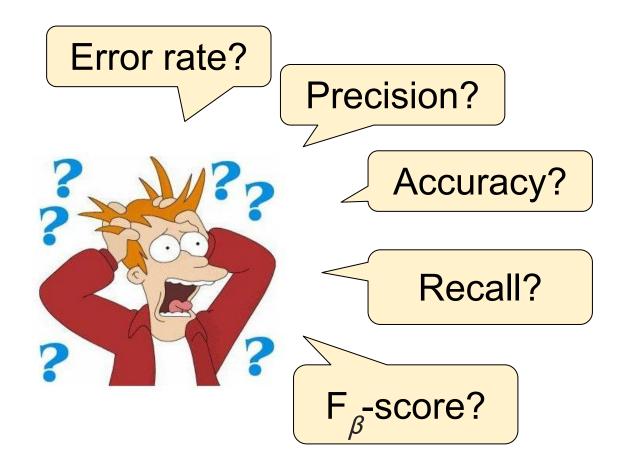


- Precision/Recall tradeoff
  - Many classifiers can be adjusted to favor precision or recall
  - Ex:Threshold based classifier













- No silver bullet
  - Best measure depends on the task being solved

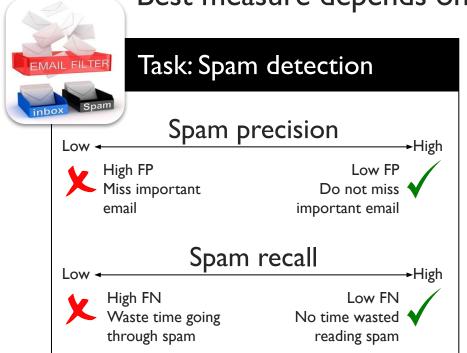




# Performance measures: classification tasks

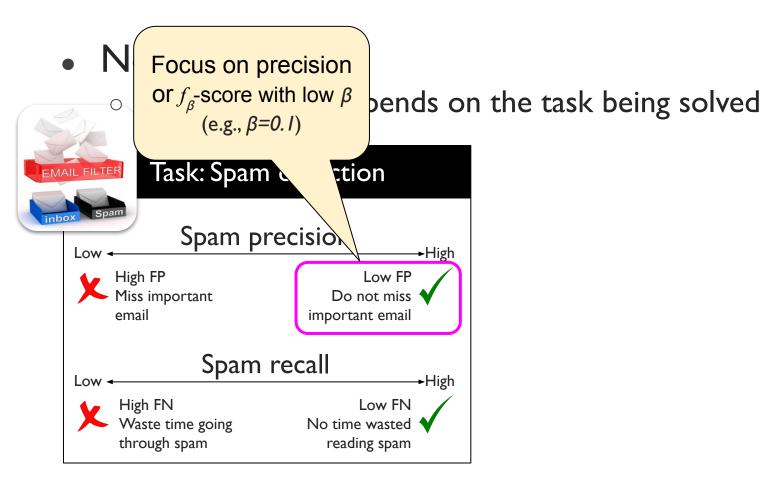
No silver bullet

Best measure depends on the task being solved







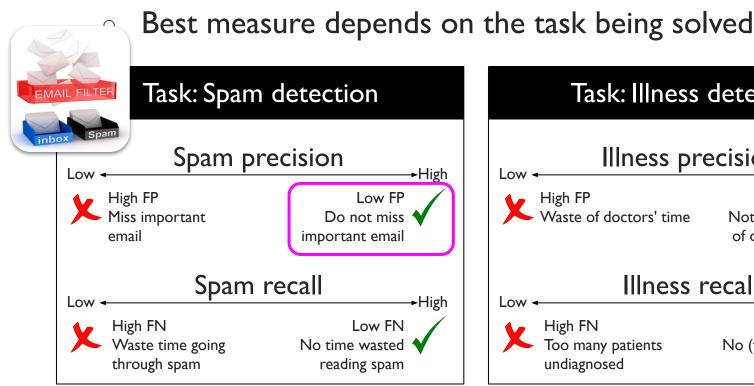


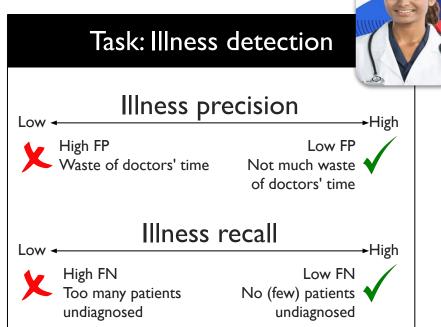




#### Performance measures: classification tasks

No silver bullet







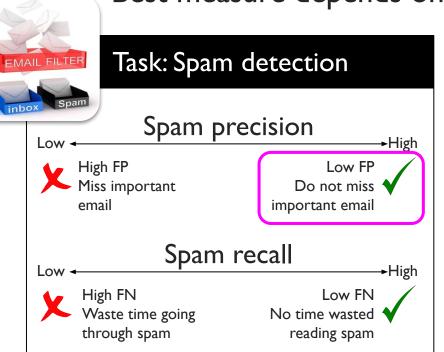


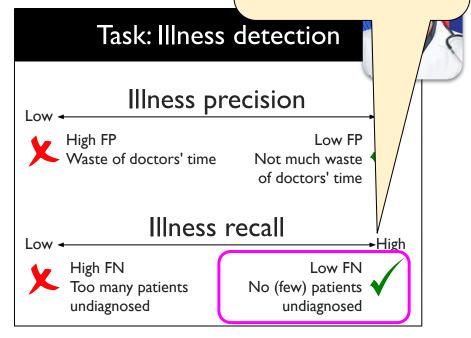
# Performance measures: classification tasks

No silver bullet

Best measure depends on the task being sol

Focus on recall or  $f_{\beta}$ -score with high  $\beta$  (e.g.,  $\beta = 10$ )









## Performance measures: classification tasks

- No silver bullet
  - Best measure depends on the task being solved



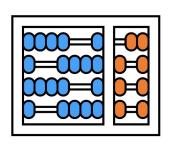


Precision

 $f_{0.5}$ -score  $f_{1}$ -score

 $f_{\gamma}$ -score

Recall



# Instituto de Computação

UNIVERSIDADE ESTADUAL DE CAMPINAS

# Capacitação profissional em tecnologias de Inteligência Artificial

# **Machine Learning Overview**

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