Model Evaluation

CS 3244 Machine Learning



IoT Sensors



Health Behavior Change



Data Analytics

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NUS Ubicomp Lab

Apps and Analytics for Smart Cities and Healthcare
http://ubiquitous.comp.nus.edu.sg



Explainable Artificial Intelligence



Interactive Data Visualization

[Instructor] Brian Lim

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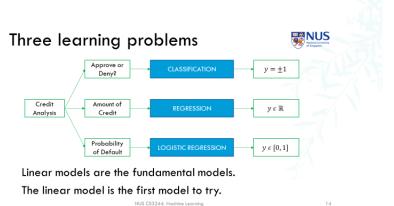
Academic Experience

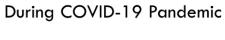
- Asst. Prof. in Computer Science
- Ph.D. in HCI, Carnegie Mellon University
- B.S. in Engineering Physics, Cornell University

Research Interests

- HCI: understand people with tech, help people with tech
- Explainable Artificial Intelligence
- Ubiquitous Computing
- Data analysis and visualization
- Smart Health and Smart Cities

Recap from Past Weeks



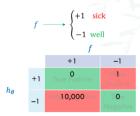


NUS Sational University of University

Are you sick?

False negative highly costly! People and the economy dies.

False positive requires the inconvenience of quarantine.



NUS CS3244: Machine Learning

W04

Analyzing the estimate

On a test point (x, y), the cost $I(h_{\theta}(x), y)$ is:

Squared error: Binary error:

$$(h_{\theta}(x) - y)^{2}$$
$$[[h_{\theta}(x) \neq y]]$$

$$\mathbb{E}[I(h_{\theta}(x), y)] = L_{test}(h_{\theta})$$

$$Var[I(h_{\theta}(x), y)] = \sigma^2$$

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Distance Metric

Often we'll use Euclidean distance as our first try:

$$L2\left(x^{(*)},x^{(i)}\right) = \sqrt{\left(x_1^{(*)} - x_1^{(i)}\right)^2 + \left(x_2^{(*)} - x_2^{(i)}\right)^2 + \dots + \left(x_n^{(*)} - x_n^{(i)}\right)^2}$$

W03

but any distance metric (non-negativity, symmetric, obeys the triangle inequality) is possible.

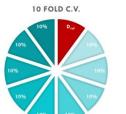
Defining your distance metric to fit your data's semantic meaning can be important.

NUS CS3744 Machine Learning



Have your cake and eat it too: *K* fold cross validation





LOOCV can be very expensive for large datasets. Why?

Instead, use K fold cross validation: i.e., K training sessions on $\frac{m}{K}$ points each.

Recommend: 10-fold CV

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W06

W02

W06

Week 07b: Learning Outcomes

- Describe various evaluation metrics of model performance
- Understand that model performance depends on prediction task and data
 - Describe several challenges in evaluating model performances
 - Choose appropriate evaluation metric for different prediction tasks

Week 07b: Lecture Outline

- 1. Recap: Supervised learning Classification vs. Regression
- 2. Classification Metrics
- 3. Regression Metrics [W08a]
- 4. Unsupervised learning metrics [W11]

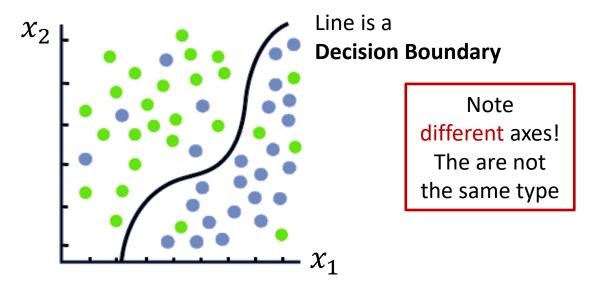


Classification vs. Regression



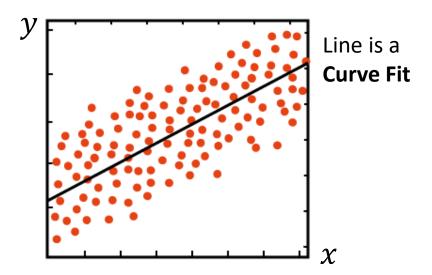
Classification

$$y \in \{0,1\}$$
 binary $y \in \{y_A, y_B, ...\}$ multi-class



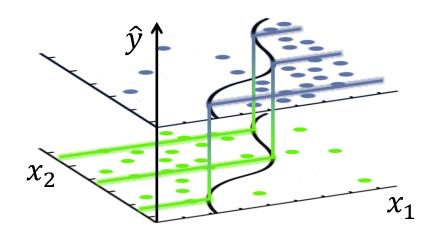
Regression

 $y \in \mathbb{R}$ any real number



Classification

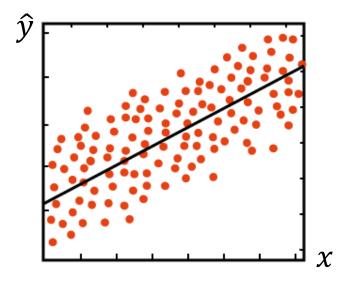
 $y \in \{0,1\}$ binary $y \in \{y_A, y_B, ...\}$ multi-class



$$y = M(x), \quad x = \vec{x} = (x_1, x_2)^{\mathsf{T}}$$

Regression

 $y \in \mathbb{R}$ any real number

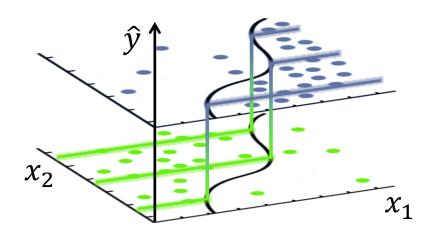


$$y = M(x), \quad x = x_1$$

Image credit:

Classification

$$y \in \{0,1\}$$
 binary $y \in \{y_A, y_B, ...\}$ multi-class



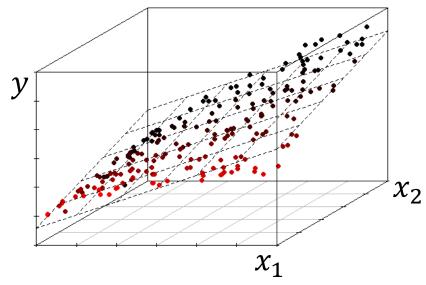
$$y = M(x), \quad x = \vec{x} = (x_1, x_2)^{\mathsf{T}}$$

Image credit:

https://www.javatpoint.com/regression-vsclassification-in-machine-learning, https://stackoverflow.com/q/26431800

Regression

 $y \in \mathbb{R}$ any real number



$$y = M(x), \quad x = x_1$$

 $y = M(x), \quad x = (x_1, ..., x_n)^{\mathsf{T}}$



Classification Evaluation Metrics



Week 07: Lecture Outline

- 1. Recap: Classification vs. Regression
- 2. Classification Metrics
 - 1. Accuracy
 - 2. Confusion Matrix, TP, TN, FP, FN
 - 3. Precision, Recall, F₁
 - 4. ROC, AUC
 - 5. Micro- and Macro-Averaging
 - 6. PR-AUC (Average Precision)
- 3. Regression Metrics [W08a]

Performance Metrics

Correctness

Classification is correct when prediction \hat{y} is the same as actual label y, i.e.,

Correct =
$$[\hat{y} = y]$$

where

- $\hat{y} = M(x)$ is the predicted value from model M instance x
- y is the ground truth value
- $[P] = \begin{cases} 1 & \text{if } P \text{ is true} \\ 0 & \text{otherwise} \end{cases}$ is the <u>Iverson bracket</u> notation for if/else

Accuracy

"Average correctness" across test dataset with m instances:

$$A = \frac{1}{m} \sum_{j=1}^{m} \left[\hat{y}_j = y_j \right]$$

where

- $\hat{y}_j = M(x_j)$ is the predicted value from model M of the jth instance x_j
- y_i is the ground truth value of the jth instance
- $[P] = \begin{cases} 1 & \text{if } P \text{ is true} \\ 0 & \text{otherwise} \end{cases}$ is the <u>Iverson bracket</u> notation for if/else

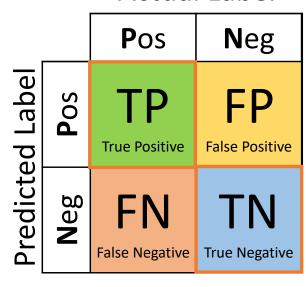
Confusion Matrix

Student alertness prediction

Inst.	Predicted \hat{y}	Actual y	
1	Alert	Alert	TD
2	Alert	Alert	TP
3	Sleepy	Alert	
4	Sleepy	Alert	FN
5	Sleepy	Alert	
6	Sleepy	Sleepy	
7	Sleepy	Sleepy	TN
8	Sleepy	Sleepy	IIN
9	Sleepy	Sleepy	
10	Alert	Sleepy	FP

Is the student **Alert**?

Actual Label



$$Accuracy = \frac{TP + TN}{TP + TN + FP + TN}$$

Confusion Matrix

Student alertness prediction

Inst.	Predicted \hat{y}	Actual y	
1	Alert	Alert	
2	Alert	Alert	
3	Sleepy	Alert	
4	Sleepy	Alert	
5	Sleepy	Alert	
6	Sleepy	Sleepy	
7	Sleepy	Sleepy	
8	Sleepy	Sleepy	
9	Sleepy	Sleepy	
10	Alert	Sleepy	

Is the student **Alert**?

Actual Label

		Pos	Neg
ed Label	Pos	TP True Positive	FP False Positive
Predicted	Neg	FN False Negative	TN True Negative

Is the student **Sleepy**?

Actual Label

		Pos	Neg
ed Label	Pos	TP True Positive	FP False Positive
Predicted	Neg	FN False Negative	TN True Negative

Which class is Positive? Negative?

You define based on your application

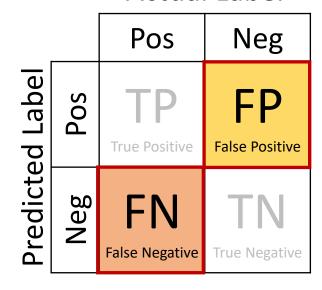
Confusion Matrix

Student alertness prediction

Inst.	Predicted \hat{y}	Actual y	
1	Alert	Alert	
2	Alert	Alert	
3	Not	Alert	
4	Not	Alert	
5	Not	Alert	
6	Not	Not	
7	Not	Not	
8	Not	Not	
9	Not	Not	
10	Alert	Not	

Is the student Alert?

Actual Label



Two types of False mistakes. Which is worse?

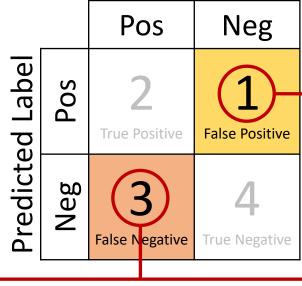
- FN: Accuse alert students, or
- FP: Neglect sleepy students?

Confusion Matrix: which mistake is costlier?

Student alertness prediction

Inst.	Predicted \hat{y}	Actual y
1	Alert	Alert
2	Alert	Alert
3	Not	Alert
4	Not	Alert
5	Not	Alert
6	Not	Not
7	Not	Not
8	Not	Not
9	Not	Not
10	Alert	Not

Actual Label



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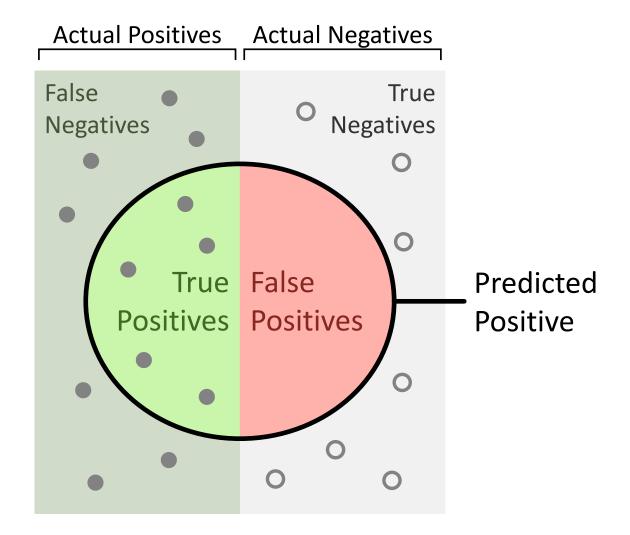
3/10 students predicted as **Sleepy** when actually **Alert**

=> Many false accusations

1/10 students predicted as **Alert** when actually **Sleepy** => Few undeserved credits

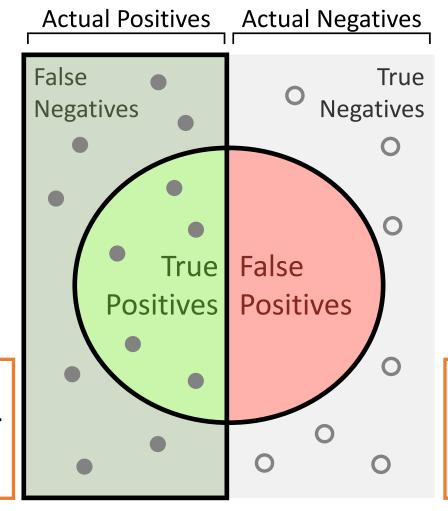
Cost-Sensitive Evaluation Metrics

- 1. Report **Precision** vs. **Recall**
- 2. Vary Prediction Threshold



What fraction of actual positive instances were recalled?

Maximize this
if false negative (FN) is costly.
E.g., cancer prediction,
not music recommendation



Among positive predictions, how **precisely** were actual positive instances predicted?

Maximize this
if false positive (FP) is costly.
E.g., email spam, satellite
launch date prediction.

Precision and Recall

Inst.	Predicted \hat{y}	Actual y
1	Alert	Alert
2	Alert	Alert
3	Not	Alert
4	Not	Alert
5	Not	Alert
6	Not	Not
7	Not	Not
8	Not	Not
9	Not	Not
10	Alert	Not

Actual Label

		Alert	Not	
Predicted Label	Alert	True Positive	Talse Positive	3 ∑ Pred. Pos.
Predicte	Not	3 False Negative	4 True Negative	\sum Pred. Neg.
·		∑ Actual Pos.	5 ∑ Actual Neg.	

Precision
P = TP / (TP+FP)

Recall
$$R = TP / (TP+FN)$$

Precision and Recall \rightarrow F₁ Score

Inst.	Predicted \hat{y}	Actual y
1	Alert	Alert
2	Alert	Alert
3	Not	Alert
4	Not	Alert
5	Not	Alert
6	Not	Not
7	Not	Not
8	Not	Not
9	Not	Not
10	Alert	Not

Actual Label

		Alert	Not	
ed Label	Alert	True Positive	1 False Positive	S Pred. Pos.
Predicted Labe	Not	3 False Negative	4 True Negative	7 ∑ Pred. Neg.
•		∑ Actual Pos.	5 ∑ Actual Neg.	

Recall
$$R = TP / (TP+FN)$$

$$F_1$$
 Score
$$F_1 = \frac{2}{4}$$

Precision

P = TP / (TP + FP)

F₁ Score: Why not just use simple average?

1. The measure is more **robust** (less sensitive to extreme values)

Ref: https://stackoverflow.com/a/26360501

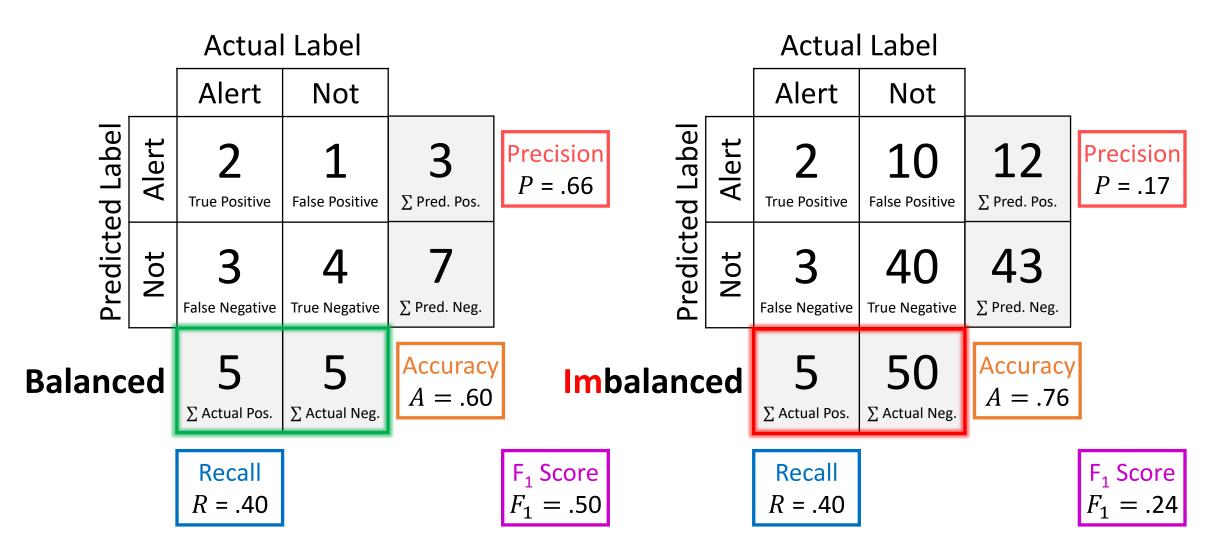
2. It considers that the numerators of P and R are the same, so it compares their denominators

$$F_1 = \left(\frac{P^{-1} + R^{-1}}{2}\right)^{-1} = \frac{2}{\frac{1}{P} + \frac{1}{R}} = \frac{2TP}{(TP + FP) + (TP + FN)}$$

Other "fairer" metrics that consider true negatives (TN):

Matthews correlation coefficient, Youden's index, Cohen's kappa

Imbalanced Data



Imbalanced Data

Actual Label

		Alert	Not		
d Label	Alert	2 True Positive	Talse Positive	3 ∑ Pred. Pos.	Precision P = .66
Predicted Label	Not	3 False Negative	4 True Negative	\sum Pred. Neg.	
		5 ∑ Actual Pos.	5 ∑ Actual Neg.	Accuracy $A = .60$	

Recall R = .40

Actual Label

		Alert	Not		
ed Label	Alert	36 True Positive	Talse Positive	37 ∑ Pred. Pos.	Precision P = .97
Predicted Label	Not	14 False Negative	4 True Negative	18 ∑ Pred. Neg.	
		50 ∑ Actual Pos.	5 ∑ Actual Neg.	Accuracy $A = .73$	<u>'</u>

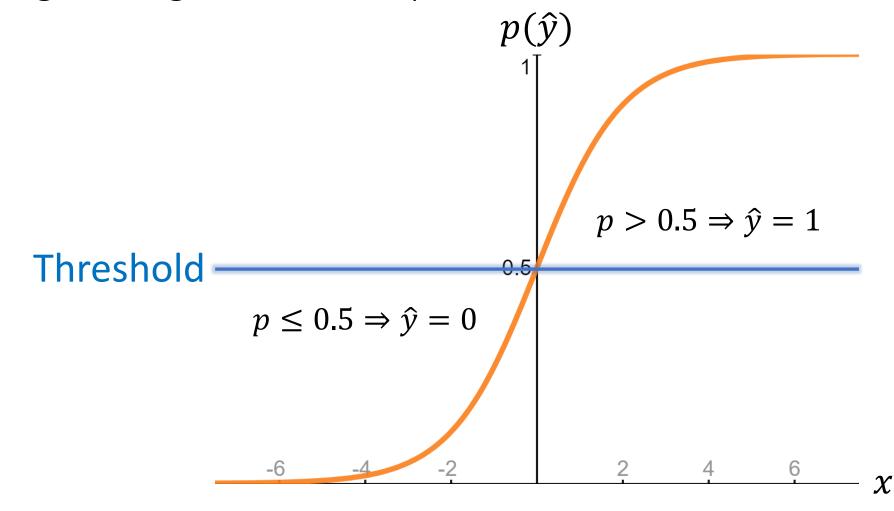
Recall R = .40

Cost-Sensitive Evaluation Metrics

- 1. Report Precision vs. Recall
- 2. Vary Prediction Threshold

Prediction Confidence

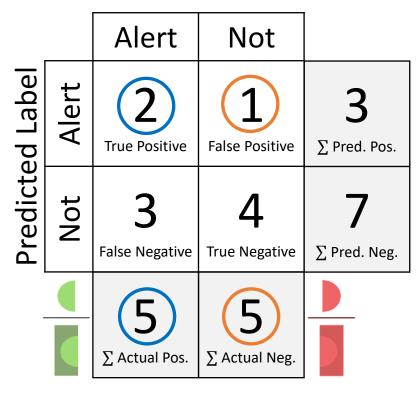
Logistic regression example



Cost-Sensitive Confusion Matrix (Threshold = **0.5**)

Inst.	Confidence $p(\hat{y})$	Prediction \hat{y} $p(\hat{y}) > 0.5$	Actual y
1	0.9	Alert	Alert
2	0.6	Alert	Alert
3	0.5	Not	Alert
4	0.4	Not	Alert
5	0.3	Not	Alert
6	0.2	Not	Not
7	0.3	Not	Not
8	0.4	Not	Not
9	0.5	Not	Not
10	0.55	Alert	Not

Actual Label



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

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

Cost-Sensitive Confusion Matrix (Threshold = **0.5**)

Inst.	Confidence $p(\hat{y})$	Prediction \hat{y} $p(\hat{y}) > 0.5$	Actual y
1	0.9	Alert	Alert
2	0.6	Alert	Alert
3	0.5	Not	Alert
4	0.4	Not	Alert
5	0.3	Not	Alert
6	0.2	Not	Not
7	0.3	Not	Not
8	0.4	Not	Not
9	0.5	Not	Not
10	0.55	Alert	Not

Actual Label

_		Alert	Not	
Predicted Label	Alert	True Positive	False Positive	3 ∑ Pred. Pos.
Predicte	Not	3 False Negative	4 True Negative	\sum Pred. Neg.
		∑ Actual Pos.	∑ Actual Neg.	

True Positive Rate TPR = 2/5 = 0.4

False Positive Rate FPR = 1/5 = 0.2

Cost-Sensitive Confusion Matrix (Threshold = **0.3**)

Inst.	Confidence $p(\hat{y})$	Prediction \hat{y} $p(\hat{y}) > 0.3$	Actual y
1	0.9	Alert	Alert
2	0.6	Alert	Alert
3	0.5	Alert	Alert
4	0.4	Alert	Alert
5	0.3	Not	Alert
6	0.2	Not	Not
7	0.3	Not	Not
8	0.4	Alert	Not
9	0.5	Alert	Not
10	0.55	Alert	Not

Actual Label

_		Alert	Not	
Predicted Label	Alert	True Positive	3 False Positive	7 ∑ Pred. Pos.
Predicte	Not	1 False Negative	2 True Negative	3 Σ Pred. Neg.
		∑ Actual Pos.	∑ Actual Neg.	

True Positive Rate TPR = 4/5 = 0.8

False Positive Rate FPR = 3/5 = 0.6

Cost-Sensitive Confusion Matrix (Threshold = **0.9**)

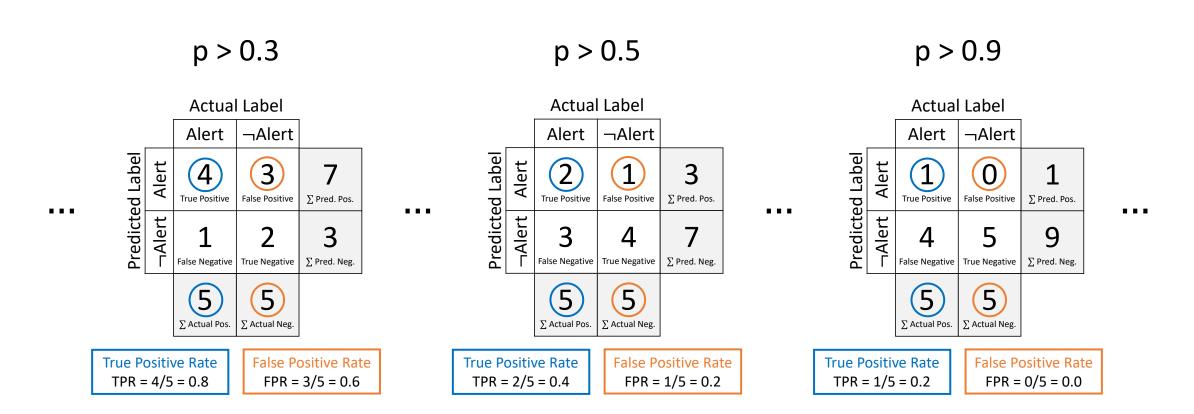
Inst.	Confidence $p(\hat{y})$	Prediction \hat{y} $p(\hat{y}) > 0.6$	Actual y
1	0.9	Alert	Alert
2	0.6	Not	Alert
3	0.5	Not	Alert
4	0.4	Not	Alert
5	0.3	Not	Alert
6	0.2	Not	Not
7	0.3	Not	Not
8	0.4	Not	Not
9	0.5	Not	Not
10	0.55	Not	Not

Actual Label

_		Alert	Not	
ed Label	Alert	True Positive	False Positive	1 Σ Pred. Pos.
Predicted Label	Not	4 False Negative	5 True Negative	9 Σ Pred. Neg.
		∑ Actual Pos.	∑ Actual Neg.	

True Positive Rate TPR = 1/5 = 0.2 False Positive Rate FPR = 0/5 = 0.0

Cost-Sensitive Confusion Matrix



Confusion matrix depends on prediction threshold

Receiver Operator Characteristic (ROC) Curve

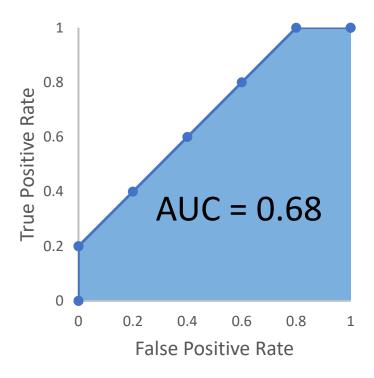
Threshold	TPR	FPR
0	1	1
0.1	1.0	1.0
0.2	1.0	0.8
0.3	0.8	0.6
0.4	0.6	0.4
0.5	0.4	0.2
0.6	0.2	0.0
0.7	0.2	0.0
0.8	0.2	0.0
0.9	0.0	0.0
1	0	0



- Diagonal random line indicates 50% chance of correctness.
- If **ROC curve** is above the **random** line, model is more accurate than chance.
- Perfect curve has TPR = 1 and FPR = 0 always.

Area Under Curve (AUC) of ROC

Threshold	TPR	FPR
0	1	1
0.1	1.0	1.0
0.2	1.0	0.8
0.3	0.8	0.6
0.4	0.6	0.4
0.5	0.4	0.2
0.6	0.2	0.0
0.7	0.2	0.0
0.8	0.2	0.0
0.9	0.0	0.0
1	0	0



- AUC is a **concise metric** instead of a full figure.
- Concise metrics enable *clearer comparisons*.
- AUC > 0.5 means the model is better than chance.
- AUC ≈ 1 means model is very accurate.

Area Under Curve (AUC) of ROC (example)

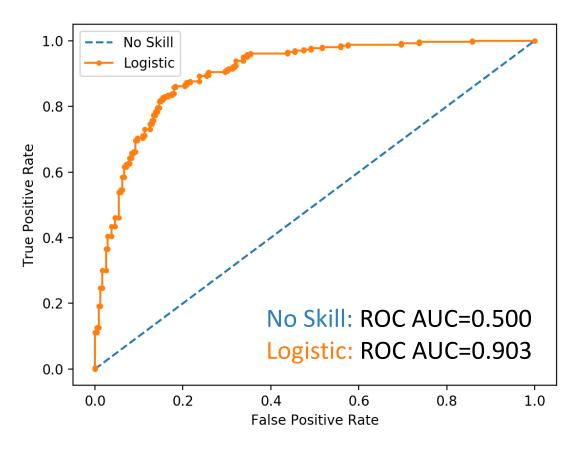


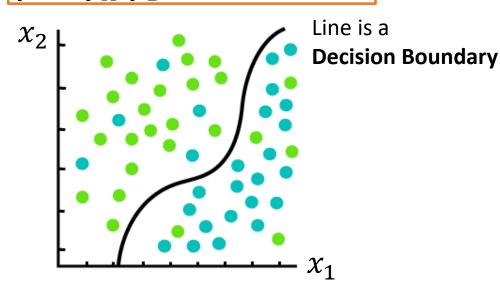
Image credit: https://machinelearningmastery.com/roc-curves-and-precision-recall-curves-for-classification-in-python/



Classification

$$\hat{y} \in \{0,1\}$$
 binary

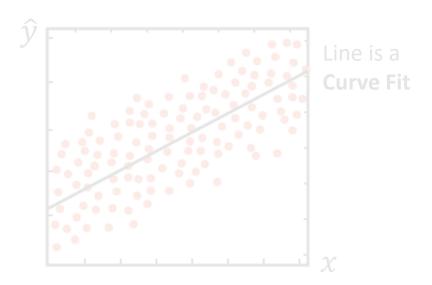
$$\hat{y} \in \{y_A, y_B, \dots\}$$
 multi-class



$$\hat{y} = M(x), \quad x = \vec{x} = (x_1, x_2)^{\mathsf{T}}$$

Regression

 $\hat{y} \in \mathbb{R}$ any real number (scalar)



$$\hat{y} = M(x), \quad x = x_1$$

 $\hat{y} = M(x), \quad x = (x_1, ..., x_n)^{\mathsf{T}}$

Image credit:

https://www.javatpoint.com/regression-vs-classification-in-machine-learning

Confusion Matrix (binary classification)

Inst.	Predicted \hat{y}	Actual y
1	Alert	Alert
2	Alert	Alert
3	Sleepy	Alert
4	Sleepy	Alert
5	Sleepy	Alert
6	Sleepy	Sleepy
7	Sleepy	Sleepy
8	Sleepy	Sleepy
9	Sleepy	Sleepy
10	Alert	Sleepy

Actual Label

		Alert	Sleepy
d Label	Alert	2	1
Predicted Label	Sleepy	3	4

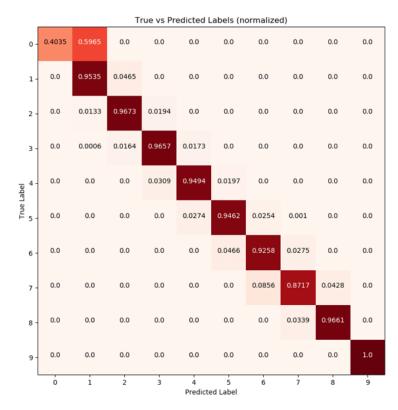
Predicted \hat{y} Actual *y* Inst. Alert Alert Alert Alert 2 Sleepy Alert Sleepy Alert 5 Sleepy Alert Sleepy 6 Sleepy Sleepy Sleepy 8 Sleepy Sleepy 9 Sleepy Sleepy 10 Alert Sleepy 11 Away Away 12 Away Alert • • • • • • • • •

Actual Label

		Alert	Sleepy	Away
pel	Alert	3	2	#
Predicted Label	Sleepy	2	3	#
Prec	Away	#	#	#

Confusion Matrix (multiclass example)

Inst.	Predicted \hat{y}	Actual y
1	Alert	Alert
2	Alert	Alert
3	Sleepy	Alert
4	Sleepy	Alert
5	Sleepy	Alert
6	Sleepy	Sleepy
7	Sleepy	Sleepy
8	Sleepy	Sleepy
9	Sleepy	Sleepy
10	Alert	Sleepy
11	Away	Away
12	Away	Alert
•••		



How to calculate:

- Accuracy
- Precision, Recall, F₁
- AUC?

Image Credit: https://www.researchgate.net/figure/Confusion-matrix-for-insample-test-predictions-Notice-the-heavily-diagonally-dominant-fig2-328997503

Confusion Matrix (binary classification)

Inst.	Predicted \hat{y}	Actual y
1	Alert	Alert
2	Alert	Alert
3	Sleepy	Alert
4	Sleepy	Alert
5	Sleepy	Alert
6	Sleepy	Sleepy
7	Sleepy	Sleepy
8	Sleepy	Sleepy
9	Sleepy	Sleepy
10	Alert	Sleepy

Actual Label

		Alert	Sleepy
d Label	Alert	2 True Positive	1 False Positive
Predicted	Sleepy	3 False Negative	4 True Negative

Predicted \hat{y} **Actual** *y* Inst. Alert Alert Alert Alert Alert Sleepy Sleepy Alert 5 Sleepy Alert 6 Sleepy Sleepy Sleepy Sleepy 8 Sleepy Sleepy 9 Sleepy Sleepy 10 Alert Sleepy 11 Away Away 12 Away Alert • • • • • • • • •

Actual Label

		Alert	Sleepy	Away
ibel	Alert	2 True Positive	1 False Positive	#
Predicted Label	Sleepy	3 False Negative	4 True Negative	#
Pre	Away	#	#	#

Which class is Positive? Negative?

Predicted \hat{y} Actual *y* Inst. Alert Alert Alert Alert Sleepy Alert Sleepy Alert Alert Sleepy Sleepy Sleepy Sleepy Sleepy Sleepy Sleepy 9 Sleepy Sleepy 10 Alert Sleepy 11 Away Away 12 Away Alert

Actual Label

		Alert	Not	Not
bel	Alert	TP	FP	FP
Predicted Label	Not	FN	TN	TN
Prec	Not	FN	TN	TN

Alert class is Positive, others Neg.

Predicted \hat{y} Actual *y* Inst. Alert Alert Alert Alert Sleepy Alert Sleepy Alert Alert Sleepy Sleepy Sleepy Sleepy Sleepy Sleepy Sleepy 9 Sleepy Sleepy 10 Alert Sleepy 11 Away Away 12 Alert Away

Actual Label

		Not	Sleepy	Not
bel	Not	TN	FN	TN
Predicted Label	Sleepy	FP	TP	FP
Pre	Not	TN	FN	TN

Sleepy class is Positive, others Neg.

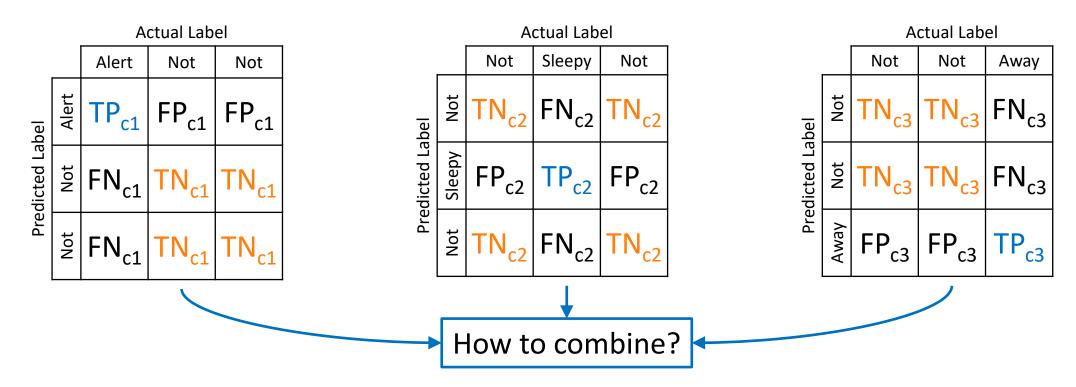
Predicted \hat{y} Actual *y* Inst. Alert Alert Alert Alert Sleepy Alert Sleepy Alert Alert Sleepy Sleepy Sleepy Sleepy Sleepy Sleepy Sleepy 9 Sleepy Sleepy 10 Alert Sleepy 11 Away Away 12 Away Alert

Actual Label

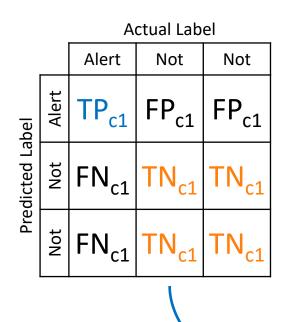
		Not	Not	Away
pel	Not	TN	TN	FN
Predicted Label	Not	TN	TN	FN
Prec	Away	FP	FP	TP

Away class is Positive, others Neg.

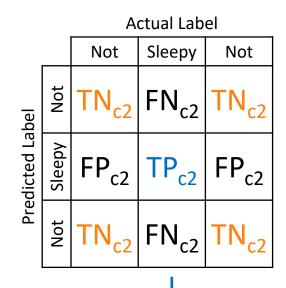
Multiclass evaluation metrics: Average?

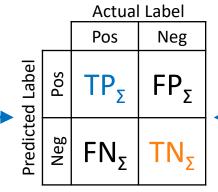


Multiclass evaluation metrics: Micro-Average



$TP_{\Sigma} = \frac{1}{ C } \sum_{c \in C} TP_c$
$= (TP_{c1} + TP_{c2} + TP_{c3})/3$
$TN_{\Sigma} = \frac{1}{ C } \sum_{c \in C} TN_c$
$FP_{\Sigma} = \frac{1}{ C } \sum_{c \in C} FP_c$
$FN_{\Sigma} = \frac{1}{ C } \sum_{c \in C} FN_c$

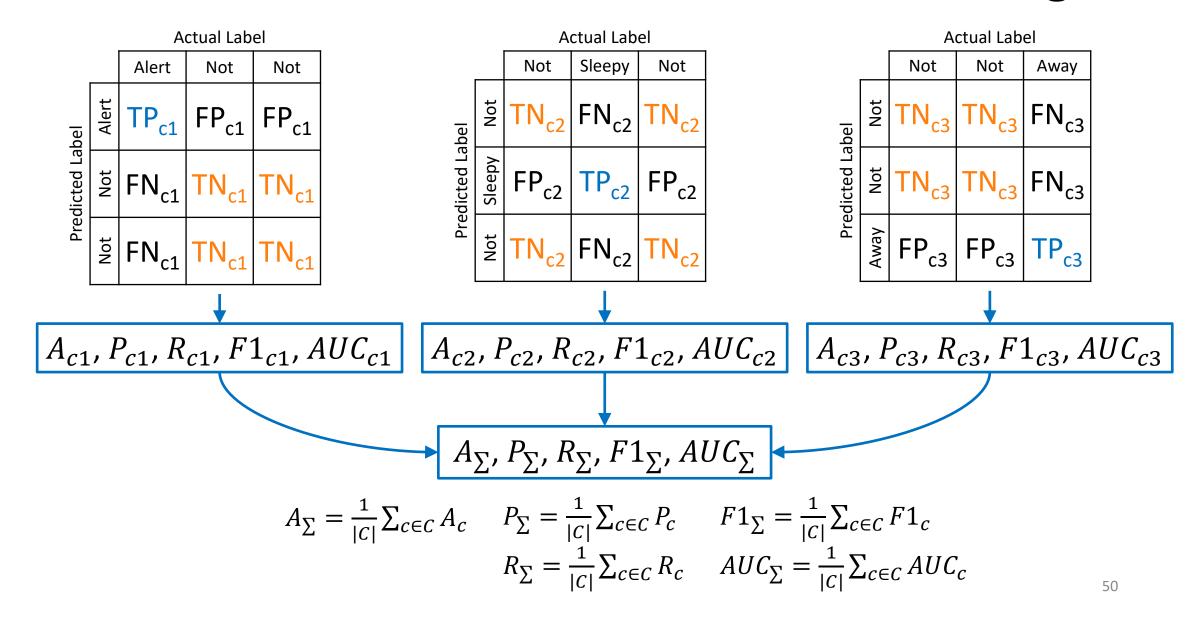




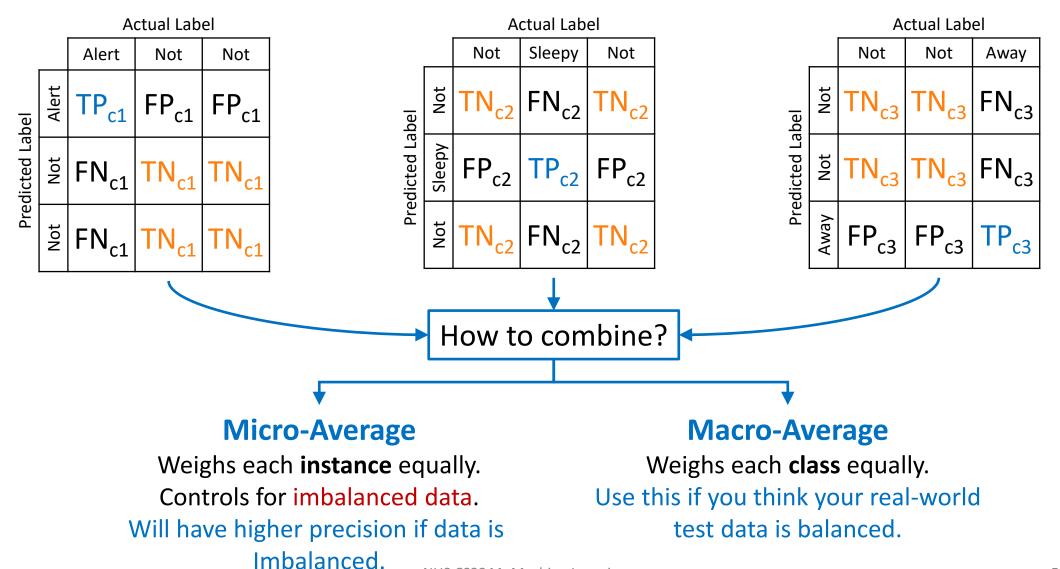
A_{Σ} ,	P_{Σ} ,	R_{Σ} ,	$F1_{\Sigma}$,	AUC_{Σ}
∠′	∠ ′	∠′	∠′	Z

		Actual Label		
Predicted Label		Not	Not	Away
	Not	TN _{c3}	TN _{c3}	FN _{c3}
	Not	TN _{c3}	TN _{c3}	FN _{c3}
	Away	FP _{c3}	FP _{c3}	TP _{c3}

Multiclass evaluation metrics: Macro-Average

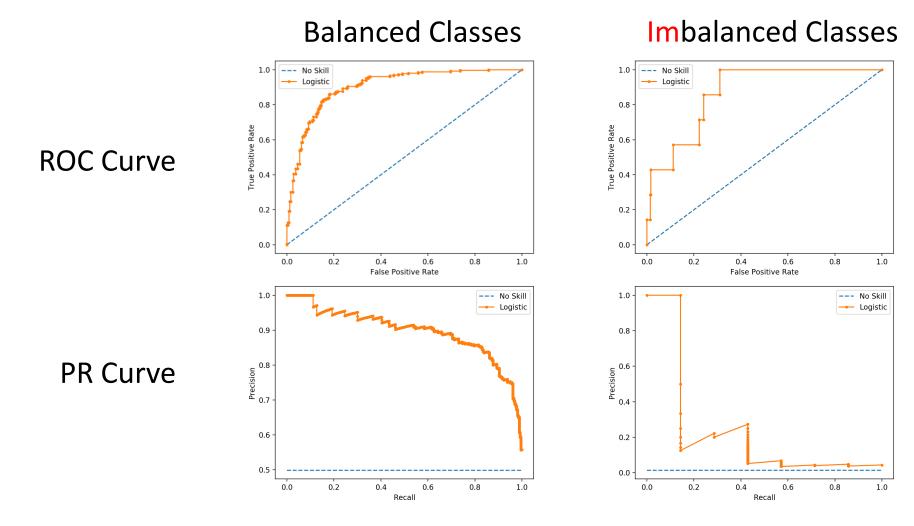


Micro- vs. Macro Average



Imbalanced Classification evaluation with Precision-Recall (PR) Curve AUC

Further reading: https://machinelearningmastery.com/roc-curves-and-precision-recall-curves-for-imbalanced-classification/



Match appropriate evaluation metric to challenge

Challenge	Evaluation Metric	
	Accuracy (Emote :one:)	
Imbalanced actual classes	Precision (:two:)	
	Recall (:three:)	
Multiclass classification	 F₁ Score (:four:) ROC AUC (:five:) PRC AUC (:six:) Micro-Average (:seven:) 	
IVIUILICIASS CIASSIIICALIOII		
Cost-dependent classes		
	Macro-Average (:eight:)	

Emote (react) in Slack #general channel one or more options (MRQ) for each challenge



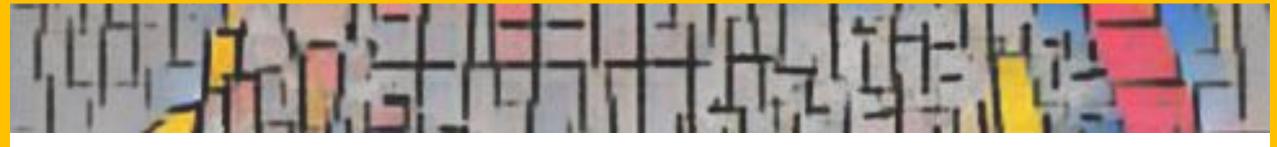
Wrapping Up



What did we learn this week?

- 1. Recap: Classification vs. Regression
- 2. Classification Metrics
 - 1. Accuracy
 - Confusion Matrix, TP, TN, FP, FN
 - 3. Precision, Recall, F₁
 - 4. ROC, AUC
 - 5. Micro- and Macro-Averaging
 - 6. PR-AUC (Average Precision)
- 3. Regression Metrics [W08a]

Performance Metrics



Regression Evaluation Metrics



Next week: Data Preparation for ML

Image credit:
https://img2.thejournal.ie/article/5047666/
river?version=5047733&width=1340

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W08 Pre-Lecture Task (due before next Mon)

Read

- 1. <u>Discover Feature Engineering, How to Engineer Features and How to Get Good</u> at It by Jason Brownlee
- 2. <u>8 Tactics to Combat Imbalanced Classes in Your Machine Learning Dataset</u> by Jason Brownlee

Task

- 1. Identify cases of bad data in machine learning
- 2. <u>Propose</u> mitigation strategies

 Tip: you can your own projects too; you don't have to be correct
- 3. Post a 1–2 sentence answer to the topic in your tutorial group: #tg-xx