Machine Learning

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https://github.com/safayani/machine_learning_course

Machine Learning

Error metrics for Imbalance classes

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Cancer classification example

Train logistic regression model $h_\theta(x)$. ($y = 1$ if cancer, $y = 0$ otherwise)

$$Accuracy = \frac{\#correctly\ classified}{\#total\ number}$$

10

Find that you got $\boxed{99\%}$ accuracy (1% error rate) on test set.

Only 0.50% of patients have cancer.

```
function y = predictCancer(x)
    y = 0; %ignore x!
return
```

1000

5

99.5% accuracy

1000 995 5

$\frac{995}{1000} = 0.995$ 99.5%

Precision/Recall

$y = 1$ in presence of rare class that we want to detect

confusion matrix

			1	0
			Actual Value (as confirmed by experiment)	
			positives	negatives
1	**Predicted Value** (predicted by the test)	positives	**TP** True Positive	**FP** False Positive
0		negatives	**FN** False Negative	**TN** True Negative

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

Precision

(Of all patients where we predicted $y = 1$, what fraction actually has cancer?)

$$Precision = \frac{TP}{TP + FP}$$

Recall

(Of all patients that actually have cancer, what fraction did we correctly detect as having cancer?)

$$Recall = \frac{TP}{TP + FN}$$

	Actual positives 1	Actual Negatives 0
Predict positives 1	0	0
Predict negatives 0	10	90

× 90 ✓ 10

$\boxed{y=0}$

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} = \frac{90}{100} \quad Precision = \frac{TP}{TP+FP} = \frac{0}{0} \quad Recall = \frac{TP}{TP+FN} = \frac{0}{10}$$

	Actual positives	Actual Negatives
Predict positives	1	0
Predict negatives	9	90

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} = \frac{91}{100} \quad Precision = \frac{TP}{TP+FP} = \frac{1}{1} \quad Recall = \frac{TP}{TP+FN} = \frac{1}{10}$$

	Actual positives 1	Actual Negatives
Predict positives 1	10	90
Predict negatives 0	0	0

$y=1$

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} = \frac{10}{100} \quad Precision = \frac{TP}{TP+FP} = \frac{10}{100} \quad Recall = \frac{TP}{TP+FN} = \frac{10}{10}$$

- **high recall + high precision** : the class is perfectly handled by the model
- **low recall + high precision** : the model can’t detect the class well but is highly trustable when it does

  Suppose we want to predict $y = 1$ (cancer) only if very confident.
- **high recall + low precision** : the class is well detected but the model also include points of other classes in it

  Suppose we want to avoid missing too many cases of cancer
- **low recall + low precision** : the class is poorly handled by the model

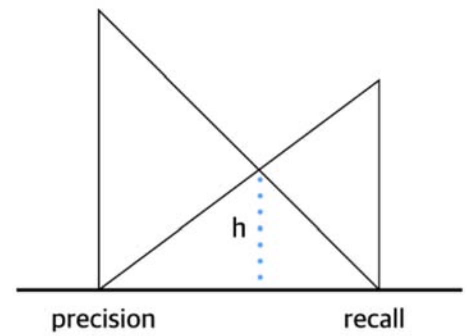
F_1 Score (F score)

How to compare precision/recall numbers?

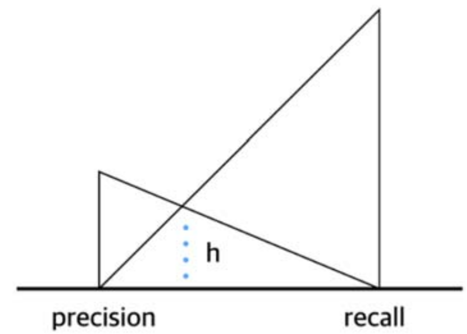
	Precision(P)	Recall (R)		
Algorithm 1	0.5	0.4	0.45	0.44
Algorithm 2	0.7	0.1	0.4	0.18
Algorithm 3	0.02	1.0	y=1 ≈ 0.5	0.04

Average: $\frac{P+R}{2}$

F_1 Score: $2\frac{PR}{P+R}$ harmonic mean



h is half the harmonic mean



Trading off precision and recall

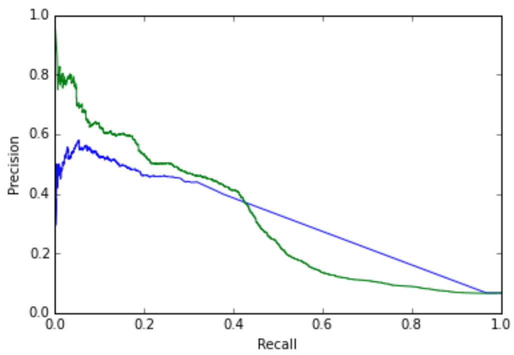
the precision-recall curve shows how the recall vs precision relationship changes as we vary the threshold for identifying a positive in our model.

$$Precision = \frac{TP}{TP + FP}$$

$$Recall = \frac{TP}{TP + FN}$$

Logistic regression: $0 \leq h_\theta(x) \leq 1$
Predict 1 if $h_\theta(x) \geq 0.5$
Predict 0 if $h_\theta(x) < 0.5$

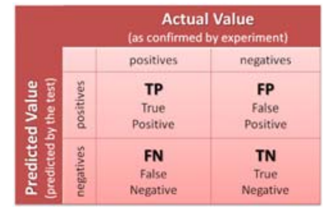
More generally: Predict 1 if $h_\theta(x) \geq$ threshold.



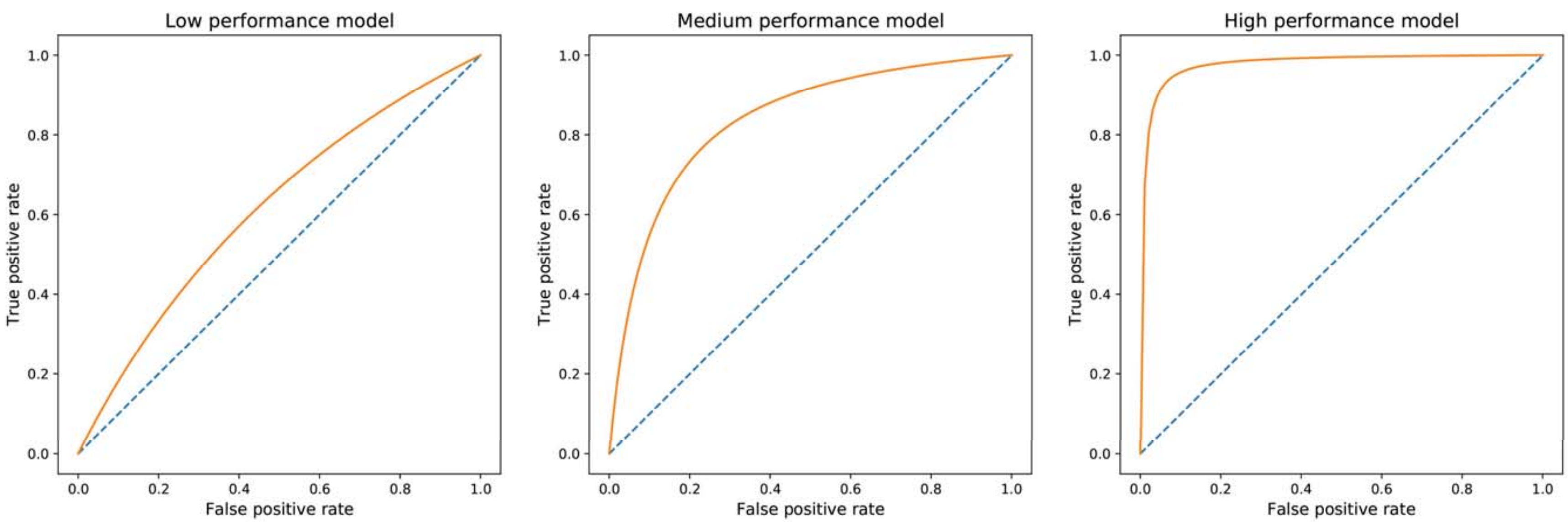
Suppose we want to predict $y = 1$ (cancer) only if very confident.
(higher threshold; higher precision; lower recall)

Suppose we want to avoid missing too many cases of cancer (avoid false negatives). (lower threshold; higher recall; lower precision)

Receiver Operating Characteristic (ROC)



$$True\ positive\ rate = \frac{TP}{TP + FN} \quad False\ positive\ rate = \frac{FP}{FP + TN}$$



F_β -Measure

$$F_\beta = \frac{(1+\beta^2) * precision * recall}{\beta^2 * precision + recall}$$

- **F0.5-Measure** (β=0.5): More weight on precision, less weight on recall.
- **F1-Measure** (β=1.0): Balance the weight on precision and recall.
- **F2-Measure** (β =2.0): Less weight on precision, more weight on recall

Multi-Class Metrics

	Actual Values				
Predictions		**A**	**B**	**C**	**D**
	A	9	1	5	0
	B	1	15	0	4
	C	0	3	24	1
	D	0	1	1	15

True Positive

	Actual Values				
Predictions		**A**	**B**	**C**	**D**
	A	9	1	5	0
	B	1	15	0	4
	C	0	3	24	1
	D	0	1	1	15

correctly identified prediction for each class

True Negative for class A

	Actual Values				
Predictions		**A**	**B**	**C**	**D**
	A	9	1	5	0
	B	1	15	0	4
	C	0	3	24	1
	D	0	1	1	15

correctly rejected prediction for certain class A

True Negative for class D

	Actual Values				
Predictions		**A**	**B**	**C**	**D**
	A	9	1	5	0
	B	1	15	0	4
	C	0	3	24	1
	D	0	1	1	15

correctly rejected prediction for certain class D

False Positive for class A

	Actual Values				
Predictions		**A**	**B**	**C**	**D**
	A	9	1	5	0
	B	1	15	0	4
	C	0	3	24	1
	D	0	1	1	15

Incorrectly identified prediction for certain class A

False Positive for class B

	Actual Values				
Predictions		**A**	**B**	**C**	**D**
	A	9	1	5	0
	B	1	15	0	4
	C	0	3	24	1
	D	0	1	1	15

Incorrectly identified prediction for certain class B

False Negative for class A

	Actual Values				
Predictions		**A**	**B**	**C**	**D**
	A	9	1	5	0
	B	1	15	0	4
	C	0	3	24	1
	D	0	1	1	15

Incorrectly rejected for certain class A

Accuracy

Accuracy is calculated as the total number of correct predictions divided by the total number of datasets

		Actual Values			
Predictions		**A**	**B**	**C**	**D**
	A	9	1	5	0
	B	1	15	0	4
	C	0	3	24	1
	D	0	1	1	15

Accuracy=(9+15+24+15)/80=0.78

Balance Data

Accuracy=32/40=0.8

		Actual Values			
Predictions		**A**	**B**	**C**	**D**
	A	10	0	0	0
	B	0	5	1	1
	C	0	3	8	0
	D	0	2	1	9

Accuracy=29/40=0.725

		Actual Values			
Predictions		**A**	**B**	**C**	**D**
	A	8	1	0	2
	B	2	7	0	3
	C	0	0	9	0
	D	0	2	1	5

Imbalance Data

Accuracy=126/230=0.547

		Actual Values			
Predictions		A	B	C	D
	A	100	0	0	0
	B	80	9	1	1
	C	10	0	8	0
	D	10	1	1	9

Accuracy=201/230=0.87

		Actual Values			
Predictions		A	B	C	D
	A	198	7	0	2
	B	2	1	8	3
	C	0	0	1	4
	D	0	2	1	1

Precision for Model 1 (Macro Average)

	Actual Values					
Predictions		**A**	**B**	**C**	**D**	
	A	100	0	0	0	TP=100 FP=0
	B	80	9	1	1	TP=9 FP=82
	C	10	0	8	0	TP=8 FP=10
	D	10	1	1	9	TP=9 FP=12

Precision=TP/(TP+FP) P(A)=1 P(B)=9/91 P(C)=8/18 P(D)=9/21

Macro Average Precision=[P(A)+P(B)+P(C)+P(D)]/4=0.492

Recall for Model 1 (Macro Average)

	Actual Values				
Predictions		**A**	**B**	**C**	**D**
	A	100	0	0	0
	B	80	9	1	1
	C	10	0	8	0
	D	10	1	1	9
		TP=100 FN=100	TP=9 FN=1	TP=8 FN=2	TP=9 FN=1

Recall=TP/(TP+FN)   R(A)=100/200   R(B)=9/10   R(C)=8/10   R(D)=9/10

Macro Average Recall=[R(A)+R(B)+R(C)+R(D)]/4=0.775

F1 Score for Model 1

	Actual Values				
Predictions		A	B	C	D
	A	100	0	0	0
	B	80	9	1	1
	C	10	0	8	0
	D	10	1	1	9

F1 Score=2*(Recall*Precision)/(Precision +Recall)

F1 Score=2*[0.492*0.775]/[0.492+0.775]=0.601

Imbalance Data

Accuracy=0.547
F1 Score=0.601

		Actual Values			
Predictions		**A**	**B**	**C**	**D**
	A	100	0	0	0
	B	80	9	1	1
	C	10	0	8	0
	D	10	1	1	9

Accuracy=0.87
F1 Score=0.342

		Actual Values			
Predictions		**A**	**B**	**C**	**D**
	A	198	7	0	2
	B	2	1	8	3
	C	0	0	1	4
	D	0	2	1	1

Learning for Imbalance Data:**Undersampling, oversampling and generating synthetic data**

•undersampling consists in sampling from the majority class in order to keep only a part of these points

•oversampling consists in replicating some points from the minority class in order to increase its cardinality

•generating synthetic data consists in creating new synthetic points from the minority class (see SMOTE method for example) to increase its cardinality

References and further readings

Andrew NG., Machine Learning Course, Coursera, slide: Error metrics for skewed classes

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Baptiste Rocca, "Handling imbalanced datasets in machine learning", 3 may 2020, https://towardsdatascience.com/handling-imbalanced-datasets-in-machine-learning-7a0e84220f28