

Machine Learning

EE514 – CS535

Analysis and Evaluation of Classifier's Performance and Multi-class Classification

$A \in \mathbb{R}^{10 \times 2}$

m -dimensional space

columns of A

Column space of A

column space of A in \mathbb{R}^m

REGRESSION: Prediction of a variable on continuous scale.

Classical
we know
- system
- output
find; input

Practice
 $x_1 + x_2 = Ax + b$

y

$f(x)$

x

System, Model Process

y

Bias

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Outline

- Classification Accuracy (0/1 Loss)
- TP, TN, FP and FN
- Confusion Matrix
- Sensitivity, Specificity, Precision Trade-offs, ROC, AUC
- F1-Score and Matthew's Correlation Coefficient
- Multi-class Classification, Evaluation, Micro, Macro Averaging

Evaluation of Classification Performance

Classification Accuracy, Misclassification Rate (0/1 Loss):

$$\mathcal{L}_{0/1}(h) = \frac{1}{n} \sum_{i=1}^n 1 - \delta_{h(\mathbf{x}_i) - y_i}$$

$$\delta_k = \begin{cases} 1, & k = 0 \\ 0 & \text{otherwise} \end{cases}$$

- For each test-point, the loss is either 0 or 1; whether the prediction is correct or incorrect.
- Averaged over n data-points, this loss is a 'Misclassification Rate'.

Interpretation:

- Misclassification Rate: Estimate of the probability that a point is incorrectly classified.
- Accuracy = 1 - Misclassification rate

Issue:

- Not meaningful when the classes are imbalanced or skewed.

Evaluation of Classification Performance

Classification Accuracy (0/1 Loss):

Example:

- Predict if a bowler will not bowl a no-ball?
 - Assuming 15 no-balls in an inning, a model that says 'Yes' all the time will have 95% accuracy.
 - Using accuracy as performance metric, we can say that a model is very accurate, but it is not useful or valuable in fact.

Why?

- Total points: 315 (assuming other balls are legal 😊)
- No-ball label: Class 0 (4.76% are from this class)
- Not a no-ball label: Class 1 (95.24% are from this class)

**Imbalanced
Classes**

Evaluation of Classification Performance

TP, TN, FP and FN:

- Consider a binary classification problem.

$$D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_n, y_n)\} \subseteq \mathcal{X}^d \times \mathcal{Y}$$

$$\mathcal{Y} = \{0, 1\} \text{ (Referring 0 as Negative, 1 as Positive)}$$

y - Actual labels, Ground truth, Gold labels or Standards

We have a classifier (hypothesis function) $h(\mathbf{x}) = \hat{y}$.

y, \hat{y} - Positive (1) or Negative (0)

\hat{y} - True if $\hat{y} = y$, False if $\hat{y} \neq y$

Evaluation of Classification Performance

TP, TN, FP and FN:

- TP - True Positive
- TN - True Negative
- FP - False Positive
- FN - False Negative
- Number of points with $y = 1$ and are classified as $\hat{y} = 1$
- Number of points with $y = 0$ and are classified as $\hat{y} = 0$
- Number of points with $y = 0$ and are classified as $\hat{y} = 1$
- Number of points with $y = 1$ and are classified as $\hat{y} = 0$

Evaluation of Classification Performance

TP, TN, FP and FN:

Example:

- Predict if a bowler will not bowl a no-ball?
 - 15 no-balls in an inning (Total balls: 315)
 - Bowl no-ball (Class 0), Bowl regular ball (Class 1)
 - Model(*) predicted 10 no-balls (8 correct predictions, 2 incorrect)

- TP - True Positive

- TP - 298

- TN - True Negative

- TN - 8

- FP - False Positive

- FP - 7

- FN - False Negative

- FN - 2

* Assume you have a model that has been observing the bowlers for the last 15 years and used these observations for learning.

Evaluation of Classification Performance

Confusion Matrix (Contingency Table):

- (TP; TN; FP; FN); usefully summarized in a table, referred to as confusion matrix:
 - the rows correspond to predicted class (\hat{y})
 - and the columns to true class (y)

		Actual Labels		Total
		1 (Positive)	0 (Negative)	
Predicted Labels	1 (Positive)	TP	FP	Predicted Total Positives
	0 (Negative)	FN	TN	Predicted Total Negatives
Total		P = TP + FN Actual Total Positives	N = P + TN Actual Total Negatives	

Evaluation of Classification Performance

Confusion Matrix:

Example:

- Disease Detection :

Given pathology reports and scans, predict heart disease

- Yes: 1, No: 0

Interpretation:

Out of 165 cases

- Predicted: "Yes" 110 times, and "No" 55 times

- In reality: "Yes" 105 times, and "No" 60 times

		Actual Labels		Total
		1 (Positive)	0 (Negative)	
Predicted Labels	1 (Positive)	TP = 100	FP = 10	110
	0 (Negative)	FN = 5	TN = 50	55
Total		P = 105	N = 60	

Evaluation of Classification Performance

Confusion Matrix:

Example:

- Predict if a bowler will not bowl a no-ball?

Interpretation:

Out of 315 balls, we had 15 no-balls.

- Model predicted 305 regular balls and 10 no-balls (8 correct predictions, 2 incorrect).

		Actual Labels		Total
		1 (Positive)	0 (Negative)	
Predicted Labels	1 (Positive)	TP = 298	FP = 7	305
	0 (Negative)	FN = 2	TN = 8	10
Total		P = 300	N = 15	

Evaluation of Classification Performance

Confusion Matrix:

Metrics using Confusion Matrix:

- *Accuracy: Overall, how frequently is the classifier correct?*

$$\text{Accuracy} = \frac{TP + TN}{\text{Total}} = \frac{TP + TN}{P + N}$$

- *Misclassification or Error Rate: Overall, how frequently is it wrong?*

$$1 - \text{Accuracy} = \frac{FP + FN}{\text{Total}} = \frac{FP + FN}{P + N}$$

- *Sensitivity or Recall or True Positive Rate (TPR): How often does it predict Positive when it is actually Positive?*

$$TPR = S_e = \frac{TP}{TP + FN} = \frac{TP}{P}$$

		Actual Labels		Total
		1 (Positive)	0 (Negative)	
Predicted Labels	1 (Positive)	TP	FP	Predicted Total Positives
	0 (Negative)	FN	TN	Predicted Total Negatives
Total		P= TP+FN Actual Total Positives	N= P+TN Actual Total Negatives	

Evaluation of Classification Performance

Confusion Matrix:

Metrics using Confusion Matrix:

- *False Positive Rate: Actual Negative, how often does it predict Positive?*

$$FPR = \frac{FP}{TN + FP} = \frac{FP}{N}$$

- *Specificity or True Negative Rate (TNR): When it's actually Negative, how often does it predict Negative?*

$$TNR = S_p = \frac{TN}{TN + FP} = \frac{TN}{N} = 1 - FPR$$

- *Precision: When it predicts Positive, how often is it Positive?*

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

		Actual Labels		Total
		1 (Positive)	0 (Negative)	
Predicted Labels	1 (Positive)	TP	FP	Predicted Total Positives
	0 (Negative)	FN	TN	Predicted Total Negatives
Total		P= TP+FN Actual Total Positives	N= P+TN Actual Total Negatives	

Evaluation of Classification Performance

Confusion Matrix Metrics:

		Actual Labels		
		1 (Positive)	0 (Negative)	
Predicted Labels	1 (Positive)	TP	FP	<i>Predicted Total Positives</i>
	0 (Negative)	FN	TN	<i>Predicted Total Negatives</i>
Total		<i>P = TP + FN Actual Total Positives</i>	<i>N = P + TN Actual Total Negatives</i>	

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

$$\frac{TN}{TN + FN} \quad \text{Negative Predicted Value}$$

$$TPR = S_e = \frac{TP}{TP + FN} = \frac{TP}{P}$$

$$TNR = S_p = \frac{TN}{TN + FP} = \frac{TN}{N}$$

Evaluation of Classification Performance

Confusion Matrix:

Metrics using Confusion Matrix (Example: Disease Prediction):

- *Accuracy: Disease/Healthy prediction accuracy*

$$\text{Accuracy} = \frac{TP + TN}{\text{Total}} = \frac{TP + TN}{P + N} = (100+50)/165 = 0.91$$

- *Misclassification or Error Rate: Disease/Healthy prediction accuracy*

$$1 - \text{Accuracy} = \frac{FP + FN}{\text{Total}} = \frac{FP + FN}{P + N} = (10+5)/165 = 0.09$$

- *Sensitivity or Recall or True Positive Rate (TPR): When it's positive, how often does the model detected disease?*

$$TPR = S_e = \frac{TP}{TP + FN} = \frac{TP}{P} = 100/105 = 0.95$$

		Actual Labels		Total
		1 (Positive)	0 (Negative)	
Predicted Labels	1 (Positive)	TP = 100	FP = 10	110
	0 (Negative)	FN = 5	TN = 50	55
Total		P = 105	N = 60	

Evaluation of Classification Performance

Confusion Matrix:

Metrics using Confusion Matrix (Example: Disease Prediction):

- *False Positive Rate: Actually healthy, how often does it predict yes?*

$$FPR = \frac{FP}{TN + FP} = \frac{FP}{N} = 10/60 = 0.17$$

- *Specificity or True Negative Rate (TNR): When it's actually health, how often does it predict healthy?*

$$TNR = S_p = \frac{TN}{TN + FP} = \frac{TN}{N} = 50/60 = 0.83$$

- *Precision: When it predicts disease, how often is it correct?*

$$\text{Precision} = \frac{TP}{TP + FP} = 100/110 = 0.91$$

		Actual Labels		Total
		1 (Positive)	0 (Negative)	
Predicted Labels	1 (Positive)	TP = 100	FP = 10	110
	0 (Negative)	FN = 5	TN = 50	55
Total		P = 105	N = 60	

Evaluation of Classification Performance

Confusion Matrix:

Metrics using Confusion Matrix:

When to use which?

- *Disease Detection: We do not want FN*

$$TPR = S_e = \frac{TP}{TP + FN} = \frac{TP}{P}$$

- *Fraud Detection: We do not want FP*

$$TNR = S_p = \frac{TN}{TN + FP} = \frac{TN}{N}$$

		Actual Labels	
		1 (Positive)	0 (Negative)
Predicted Labels	1 (Positive)	TP	FP
	0 (Negative)	FN	TN

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

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Evaluation of Classification Performance

Confusion Matrix:

Precision and Sensitivity (Recall) Trade-off:

- Disease Detection:

Sensitivity or Recall

$$TPR = S_e = \frac{TP}{TP + FN} = \frac{TP}{P}$$

Precision

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

- **Recall or Sensitivity (S_e)**; how good we are at detecting **diseased** people.

- **Precision**: How many have been correctly diagnosed as unhealthy.

- If we have diagnosed everyone unhealthy, $S_e=1$ (diagnose all unhealthy people correctly) but Precision may be low (because $TN=0$ that increases the value of FP).

		Actual Labels	
		1 (Positive)	0 (Negative)
Predicted Labels	1 (Positive)	TP	FP
	0 (Negative)	FN	TN

- We want high Precision and high S_e ($=1$, **Ideally**).

- **We should combine precision and sensitivity to evaluate the performance of classifier.**

- **F1-Score**

Evaluation of Classification Performance

Confusion Matrix:

Sensitivity and Specificity Trade-off:

- Disease Detection:
 - $$TPR = S_e = \frac{TP}{TP + FN} = \frac{TP}{P}$$
 - $$TNR = S_p = \frac{TN}{TN + FP} = \frac{TN}{N}$$
- S_p and S_e ; how good we are at detecting **healthy** and **diseased** people, respectively.
- If we have diagnosed everyone healthy, $S_p=1$ (diagnose all healthy people correctly) but $S_e=0$ (diagnose all unhealthy people incorrectly)
- **Ideally:** we want $S_p = S_e = 1$ (perfect sensitivity and specificity) but unrealistic.

Evaluation of Classification Performance

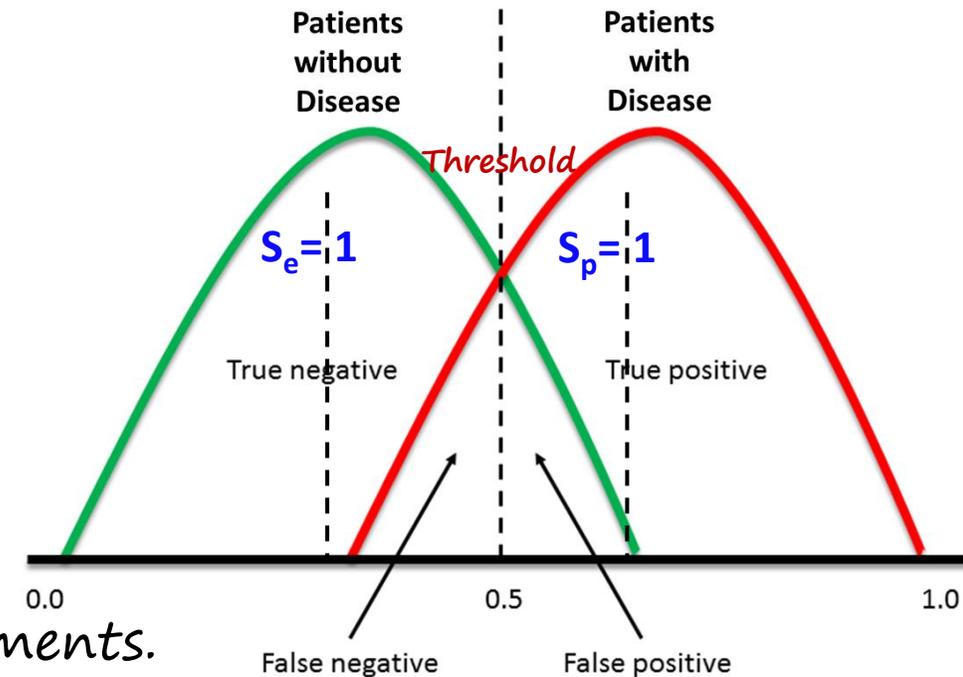
Confusion Matrix:

Sensitivity and Specificity Trade-off:

$$TNR = S_p = \frac{TN}{TN + FP} = \frac{TN}{N} \quad TPR = S_e = \frac{TP}{TP + FN} = \frac{TP}{P}$$

How optimal a pair of sensitivity, specificity values is?

- Is $S_p = 0.8, S_e = 0.7$ better than $S_p = 0.7, S_e = 0.8$?
- The answer depends on the application.
- In disease diagnosis;
 - happy to reduce S_p in order to increase S_e .
- In other applications, we may have different requirements.
- Trade-off is better explained by ROC curve and AUC.

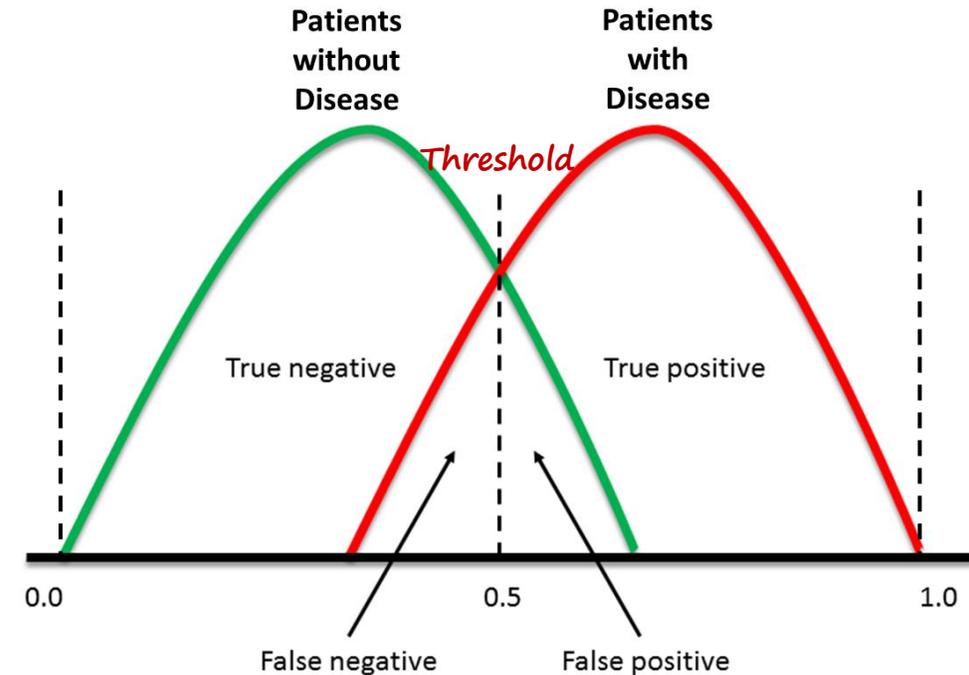


Evaluation of Classification Performance

Confusion Matrix:

ROC (Receiver Operating Characteristic) Curve:

- Plot of TPR (Sensitivity) against FPR (1 - Specificity) for different values of threshold.
- Also referred to as Sensitivity-(1-Specificity) plot.
- Threshold of 0.0, every case is diagnosed as positive.
 - $S_e = \text{TPR} = 1$
 - $\text{FPR} = 1$
 - $S_p = 0$
- Threshold of 1.0, every case is diagnosed as negative.
 - $S_e = \text{TPR} = 0$
 - $\text{FPR} = 0$
 - $S_p = 1$



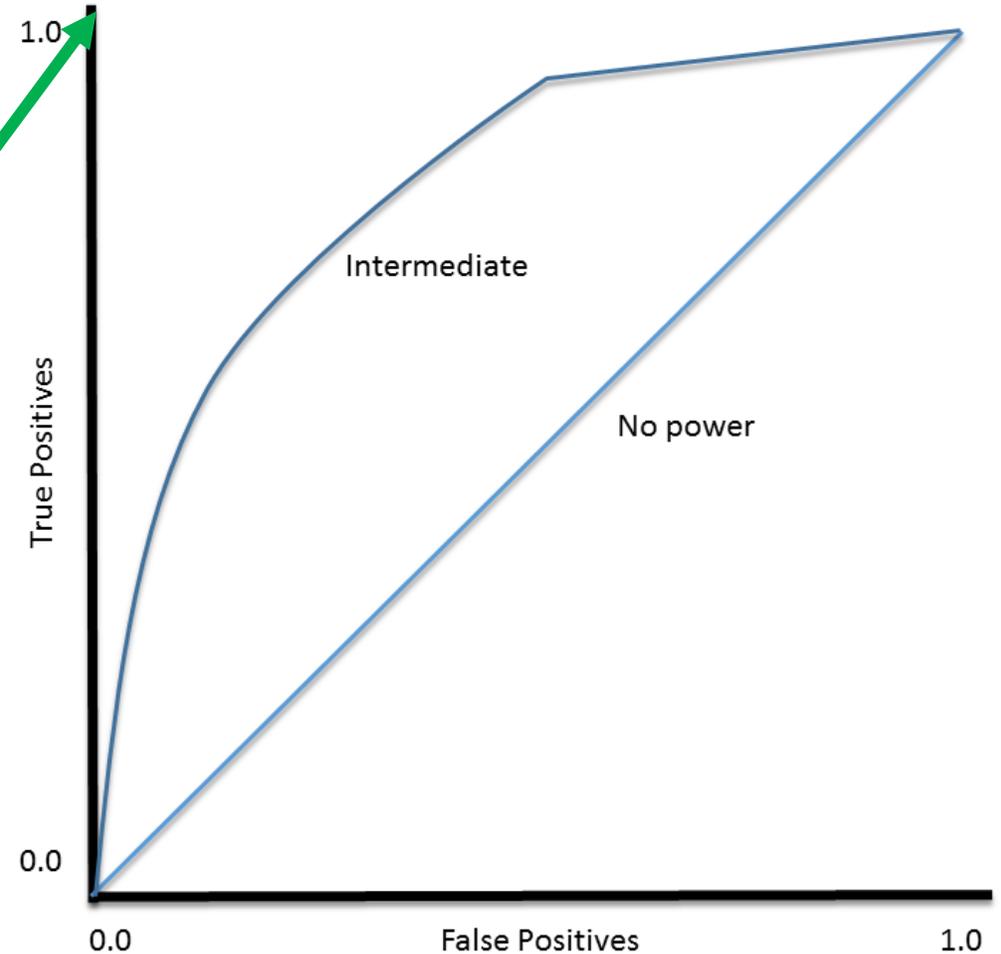
Evaluation of Classification Performance

Confusion Matrix:

ROC Curve and AUC:

- TPR (Sensitivity): how many correct positive results occur among all positive samples.
- FPR ($1 - \text{Specificity}$): how many incorrect positive results occur among all negative samples.
- The best possible prediction method
 - $S_e = S_p = 1$ (Upper left corner of ROC space)
- Random guess; a point along a diagonal line (the so-called line of no-discrimination), No Power!
- Area Under the ROC Curve, abbreviated as (AUC) quantifies the power of the classifier.

ROC Curve



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Evaluation of Classification Performance

F1-Score:

- We observed trade-off between recall and precision.

$$TPR = S_e = \frac{TP}{TP + FN} = \frac{TP}{P} \quad \text{Precision} = \frac{TP}{TP + FP}$$

- Higher levels of recall may be obtained at the price of lower values of precision.
- We need to define a single measure that combines recall and precision or other metrics to evaluate the performance of a classifier.
- Some combined measures:
 - F1 Score
 - Matthew's Correlation Coefficient
 - 11-point average precision
 - The Breakeven point

Evaluation of Classification Performance

F1 Score:

- One measure that assesses recall and precision trade-off is weighted harmonic mean (HM) of recall and precision, that is,

$$F_{\beta} = \frac{1 + \beta^2}{\frac{1}{\text{Precision}} + \frac{\beta^2}{\text{Recall}}}, \quad \beta \geq 0$$

For $\beta = 1$, we have harmonic mean of precision and recall, that is,

$$F_1 = \frac{2}{\frac{1}{\text{Precision}} + \frac{1}{\text{Recall}}} = \frac{2(\text{Precision})(\text{Recall})}{(\text{Precision}) + (\text{Recall})} = \frac{2\text{TP}}{2\text{TP} + \text{FP} + \text{FN}}$$

Evaluation of Classification Performance

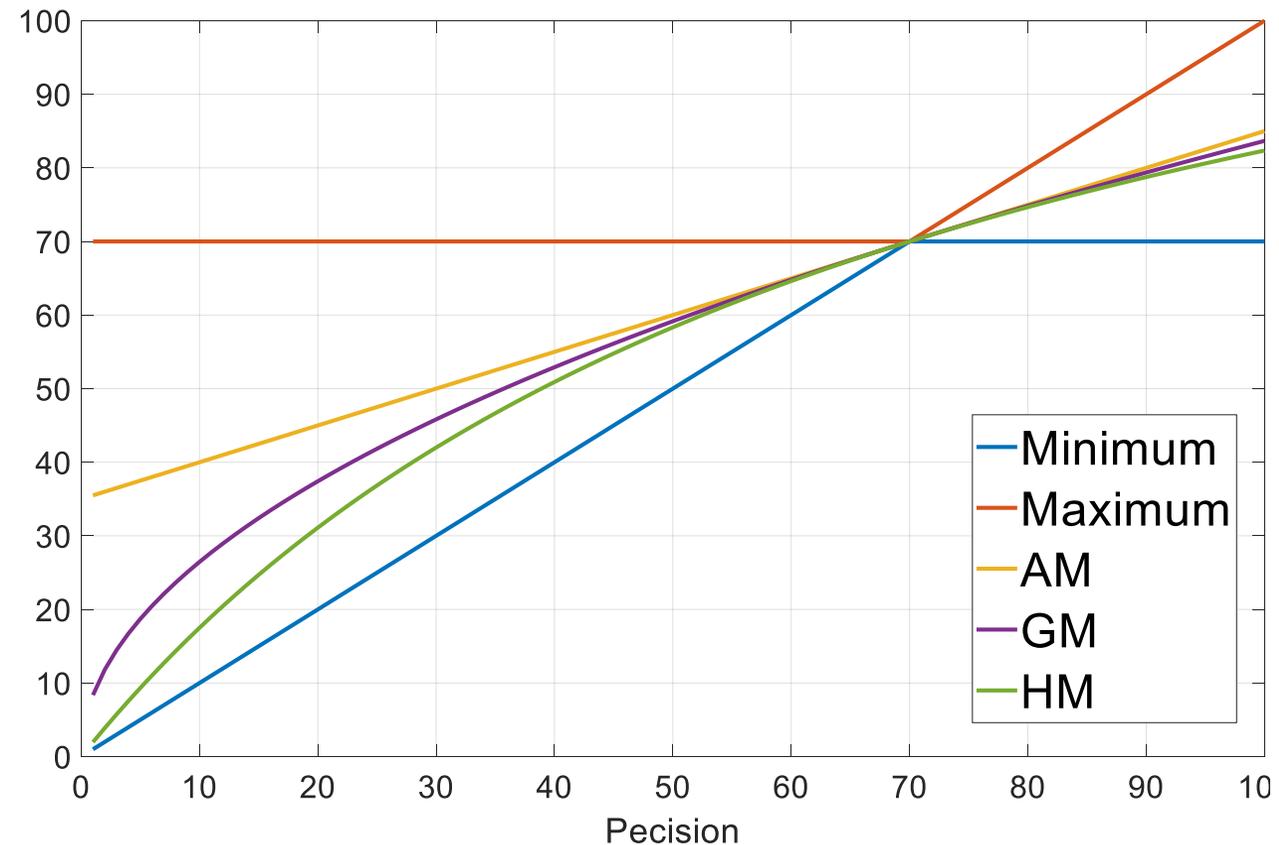
F1 Score:

Why harmonic mean?

- We could also use arithmetic mean (AM) or geometric mean (GM).
- HM is preferred as it penalizes model the most; a conservative average, that is, for two real positive numbers, we have

$$HM \leq GM \leq AM$$

- Improvement in HM implies improvement in AM or GM.



Different means, minimum and maximum against precision. Recall=70% is fixed.

Evaluation of Classification Performance

Matthew's Correlation Coefficient (MCC):

- Precision, Recall and F1-score are asymmetric. Get a different result if the classes are switched.
- Matthew's correlation coefficient determines the correlation between true class and predicted class. The higher the correlation between true and predicted values, the better the prediction.
- Defined as
$$\text{MCC} = \frac{(\text{TP})(\text{TN}) - (\text{FP})(\text{FN})}{\sqrt{(\text{TP} + \text{FN})(\text{TP} + \text{FP})(\text{TN} + \text{FN})(\text{TN} + \text{FP})}}, \quad |\text{MCC}| \leq 1$$
- $\text{MCC}=1$ when $\text{FP} = \text{FN} = 0$ (Perfect classification)
- $\text{MCC}=-1$ when $\text{TP} = \text{TN} = 0$ (Perfect misclassification)
- $\text{MCC}=0$; Performance of classifier is not better than a random classifier (flip coin)
- MCC is symmetric by design

Evaluation of Classification Performance

11-point Average Precision:

- Adjust threshold of the classifier such that the recall takes the following 11 values 0.0, 0.1., ..., 0.9, 1.0.
- For each value of the recall, determine the precision and find the average value of precision, referred to as average precision (AP).
- This is just uniformly-spaced sampling of Precision-Recall curve and taking average value.

The Breakeven Point:

- Compute precision as a function of recall for different values of thresholds.
- When Precision = Recall, we have a breakeven.

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Multi-Class Classification

Formulation:

- We assume we have training data D given by

$$D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_n, y_n)\} \subseteq \mathcal{X}^d \times \mathcal{Y}$$

- $\mathcal{Y} = \{1, 2, \dots, M\}$ (M-class classification)

Examples:

- *Emotion Detection.*
- *Vehicle Type, Make, model, color of the vehicle from the images streamed by safe city camera.*
- *Speaker Identification from Speech Signal.*
- *State (rest, ramp-up, normal, ramp-down) of the process machine in the plant.*
- *Sentiment Analysis (Categories: Positive, Negative, Neutral), Text Analysis.*
- *Take an image of the sky and determine the pollution level (healthy, moderate, hazard).*
- *Record Home WiFi signals and identify the type of appliance being operated.*



Multi-Class Classification

Implementation (Possible options using binary classifiers):

Option 1: Build a one-vs-all (OvA) one-vs-rest (OvR) classifier:

Train M different binary classifiers $h_1(\mathbf{x}), h_2(\mathbf{x}), \dots, h_M(\mathbf{x})$.

Classifier $h_i(\mathbf{x})$ is trained to classify if \mathbf{x} belongs to i -th class or not.

For a new test point \mathbf{z} , get scores for each classifier, that is, $s_i = h_i(\mathbf{z})$.

For example, s_i can be assigned the probability that \mathbf{z} belongs to class i .

Predict the label as $\hat{y} = \max_{i=1,2,\dots,M} s_i$

Option 2: Build an all-vs-all classifier:

Train $\binom{M}{2} = \frac{(M)(M-1)}{2}$ different binary classifiers $h_{i,j}(\mathbf{x}), i, j = 1, 2, \dots, k$

Classifier $h_{i,j}(\mathbf{x})$ is trained to classify if \mathbf{x} belongs to i -th class or j -th class.

For a new test point \mathbf{z} , get scores for each classifier, that is, $s_{i,j} = h_{i,j}(\mathbf{z})$. For example, $s_{i,j} = 1$ if \mathbf{z} is likely class i or 0 if \mathbf{z} is likely class j .

Predict the label \hat{y} that has been predicted multiple times.

There can be other options...

Evaluation of Classification Performance

Multiclass Classification:

- *How do we define the measures for the evaluation of the performance of multi-class classifier?*
- *Macro-averaging: We compute performance for each class and then average.*
- *Micro-averaging: Compute confusion matrix after collecting decisions for all classes and then evaluate.*

Evaluation of Classification Performance

Multiclass Classification:

Confusion Matrix

- Predict if a bowler will bowl a no-ball, wide bowl, regular bowl?
 - 15 no-balls, 20 wide-balls in an inning (Total balls: 335)
 - Model Predictions:

		<i>Actual</i>			<i>Precision</i>
		No-ball	Wide-ball	Regular ball	
<i>Classifier Output</i>	No-ball	8	5	20	$\frac{8}{8+5+20}$
	Wide-ball	2	10	10	$\frac{10}{2+10+10}$
	Regular ball	5	5	270	$\frac{270}{5+5+270}$
<i>Recall</i>		$\frac{8}{8+2+5}$	$\frac{10}{5+10+5}$	$\frac{270}{20+10+270}$	

Evaluation of Classification Performance

Multiclass Classification:

Confusion Matrix – Recall and Precision:

$C_{i,j}$ represents the entry of the confusion matrix at i -th row and j -th column.

Recall

- For i -th class, recall represents the fraction of data-points classified correctly, that is,

$$\text{Recall}_i = \frac{C_{i,i}}{\sum_{j=1}^M C_{j,i}}$$

Precision

- For i -th class, precision represents the fraction of data-points predicted to be in class i are actually in the i -th class, that is,

$$\text{Precision}_i = \frac{C_{i,i}}{\sum_{j=1}^M C_{i,j}}$$

Accuracy

- Fraction of data points classified correctly, that is,

$$\text{Accuracy} = \frac{\sum_{i=1}^M C_{i,i}}{\sum_{i=1}^M \sum_{j=1}^M C_{i,j}}$$

	No-ball	Wide-ball	Regular ball
No-ball	8	5	20
Wide-ball	2	10	10
Regular ball	5	5	270

Evaluation of Classification Performance

Multiclass Classification:

Confusion Matrix – Macro-Averaging:

- We compute performance for each class and then average.

Confusion Matrix – Each Class:

	No-ball	Wide-ball	Regular ball
No-ball	8	5	20
Wide-ball	2	10	10
Regular ball	5	5	270

		Actual	
		No-ball	Not a No-ball
Classifier Output	No-ball	8	25
	Not a no-ball	7	295

Recall

$$\frac{8}{8+7} = 0.53$$

		Actual	
		Wide	Not Wide
Classifier Output	Wide	10	12
	Not Wide	10	303

$$\frac{10}{20} = 0.50$$

		Actual	
		Regular	Not Regular
Classifier Output	Regular	270	10
	Not Regular	30	25

$$\frac{270}{300} = 0.90$$

Macro-average Recall: $\frac{0.53+0.50+0.90}{3} = 0.64$

Evaluation of Classification Performance

Multiclass Classification:

Confusion Matrix – Micro-Averaging:

- Compute confusion matrix after collecting decisions for all classes and then evaluate.

	True	False
True	288	47
False	47	623

Micro-average

Recall:

$$\frac{288}{335} = 0.86$$

Confusion Matrix – Each Class:

		Actual	
		No-ball	Not a No-ball
Classifier Output	No-ball	8	25
	Not a no-ball	7	295

		Actual	
		Wide	Not Wide
Classifier Output	Wide	10	12
	Not Wide	10	303

		Actual	
		Regular	Not Regular
Classifier Output	Regular	270	10
	Not Regular	30	25

Evaluation of Classification Performance

Multiclass Classification:

Micro-Averaging vs Macro Averaging:

- Note Micro-average recall = Micro-average precision = F1 Score = Accuracy (computed from confusion matrix)
 - Micro-average is termed as a global metric.
 - Consequently, it is not a good measure when classes are not balanced.
- Macro-average is relatively a better as we can see a zoomed-in picture before averaging.
- Note Macro-averaging does not take class imbalance into account.
 - **Weighted-averaging**; Similar to Macro averaging but takes a weighted mean instead where weight for each class is the total number of data-points of that class.

Weighted-average Recall:
$$\frac{(15 \times 0.53) + (20 \times 0.50) + (300 \times 0.90)}{15 + 20 + 300} = 0.86$$

Feedback: Questions or Comments?

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