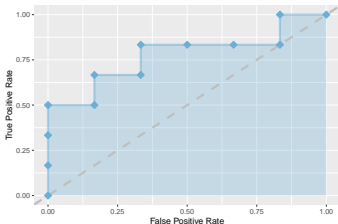


Introduction to Machine Learning

Evaluation: Measures for Binary Classification: ROC Visualization

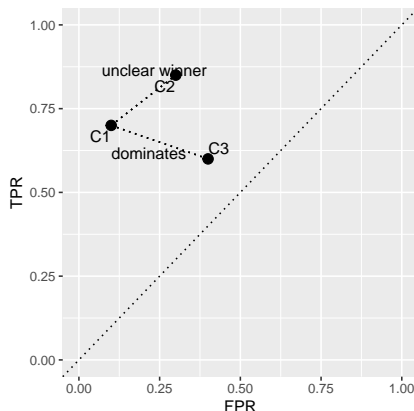


Learning goals

- Understand the ROC curve
- Be able to compute a ROC curve manually

LABELS: ROC SPACE

- We characterize a classifier by its TPR and FPR values and plot them in a coordinate system.
- We could also use two different ROC metrics which define a trade-off, for instance, TPR and PPV.



		True Class y	
		+	-
Pred. \hat{y}	+	TP	FP
	-	FN	TN

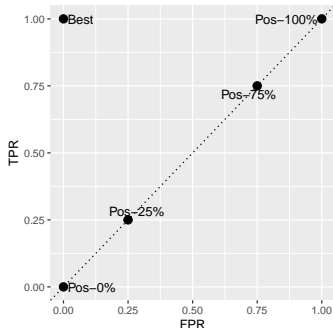
$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

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

LABELS: ROC SPACE

- The best classifier lies on the top-left corner, where FPR equals 0 and TPR is maximal.
- The diagonal is worst as it corresponds to a classifier producing random labels (with different proportions).

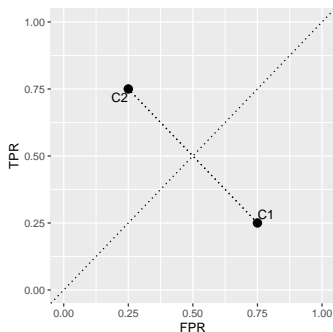
- If each positive x will be randomly classified with 25% as "pos", $TPR = 0.25$.
- If we assign each negative x randomly to "pos", $FPR = 0.25$.



LABELS: ROC SPACE

- In practice, we should never obtain a classifier below the diagonal.
- Inverting the predicted labels ($0 \mapsto 1$ and $1 \mapsto 0$) will result in a reflection at the diagonal.

$\Rightarrow \text{TPR}_{\text{new}} = 1 - \text{TPR}$ and $\text{FPR}_{\text{new}} = 1 - \text{FPR}$.



LABEL DISTRIBUTION IN TPR AND FPR

TPR and FPR (ROC curves) are insensitive to the class distribution in the sense that they are not affected by changes in the ratio n_+/n_- (at prediction).

Example 1:

Proportion $n_+/n_- = 1$

	Actual Positive	Actual Negative
Pred. Positive	40	25
Pred. Negative	10	25

$$\text{MCE} = 35/100 = 0.35$$

$$\text{TPR} = 0.8$$

$$\text{FPR} = 0.5$$

Example 2:

Proportion $n_+/n_- = 2$

	Actual Positive	Actual Negative
Pred. Positive	80	25
Pred. Negative	20	25

$$\text{MCE} = 45/150 = 0.3$$

$$\text{TPR} = 0.8$$

$$\text{FPR} = 0.5$$

Note: If class proportions differ during training, the above is not true.
Estimated posterior probabilities can change!

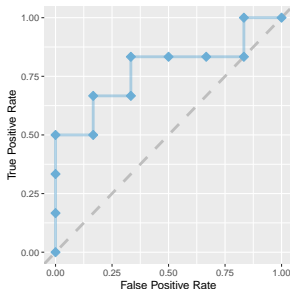
FROM PROBABILITIES TO LABELS: ROC CURVE

Remember: Both probabilistic and scoring classifiers can output classes by thresholding:

$$h(\mathbf{x}) = [\pi(\mathbf{x}) \geq c] \quad \text{or} \quad h(\mathbf{x}) = [f(\mathbf{x}) \geq c].$$

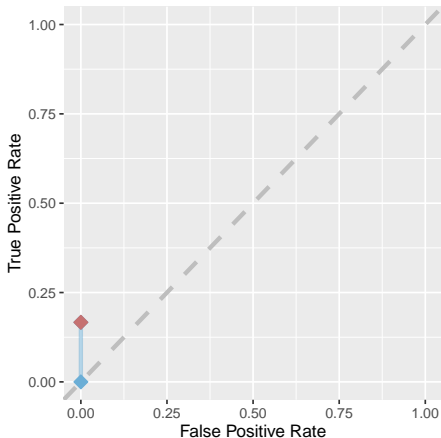
To draw a ROC curve:

- ❶ Rank test observations on decreasing score.
- ❷ Start with $c = 1$, so we start in $(0, 0)$; we predict everything as negative.
- ❸ Iterate through all possible thresholds c and proceed for each observation x as follows:
 - If x is positive, move TPR $1/n_+$ up,
 - as we have one TP more.
 - If x is negative, move FPR $1/n_-$ right,
 - as we have one FP more.



DRAWING ROC CURVES

#	Truth	Score
1	Pos	0.95
2	Pos	0.86
3	Pos	0.69
4	Neg	0.65
5	Pos	0.59
6	Neg	0.52
7	Pos	0.51
8	Neg	0.39
9	Neg	0.28
10	Neg	0.18
11	Pos	0.15
12	Neg	0.06



$$c = 0.9$$

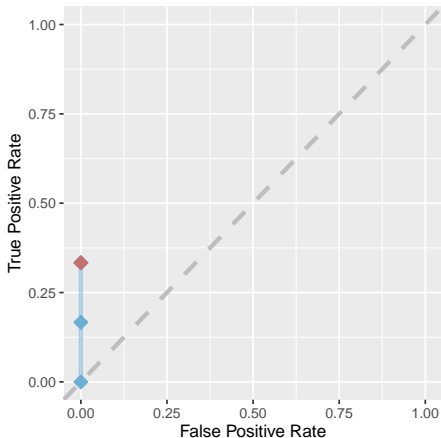
$$\rightarrow \text{TPR} = 0.167$$

$$\rightarrow \text{FPR} = 0$$

add plot showing sliding thresholds (suggestion Ludwig)

DRAWING ROC CURVES

#	Truth	Score
1	Pos	0.95
2	Pos	0.86
3	Pos	0.69
4	Neg	0.65
5	Pos	0.59
6	Neg	0.52
7	Pos	0.51
8	Neg	0.39
9	Neg	0.28
10	Neg	0.18
11	Pos	0.15
12	Neg	0.06



$$c = 0.85$$

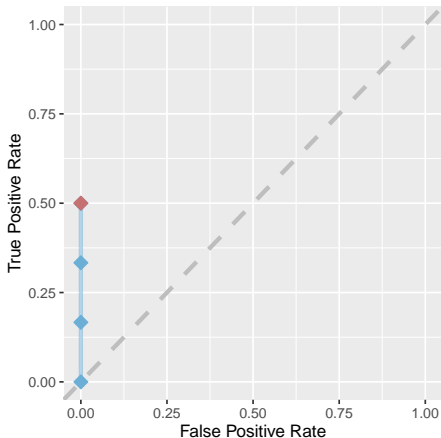
$$\rightarrow \text{TPR} = 0.333$$

$$\rightarrow \text{FPR} = 0$$

add plot showing sliding thresholds (suggestion Ludwig)

DRAWING ROC CURVES

#	Truth	Score
1	Pos	0.95
2	Pos	0.86
3	Pos	0.69
4	Neg	0.65
5	Pos	0.59
6	Neg	0.52
7	Pos	0.51
8	Neg	0.39
9	Neg	0.28
10	Neg	0.18
11	Pos	0.15
12	Neg	0.06



$$c = 0.66$$

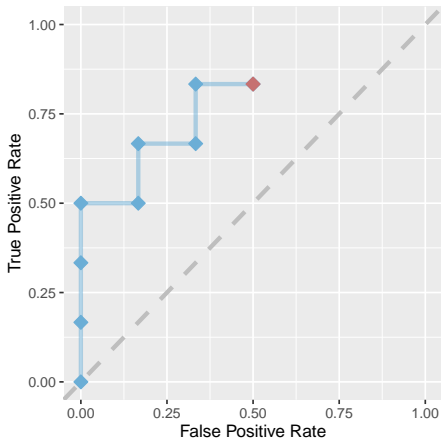
$$\rightarrow \text{TPR} = 0.5$$

$$\rightarrow \text{FPR} = 0$$

add plot showing sliding thresholds (suggestion Ludwig)

DRAWING ROC CURVES

#	Truth	Score
1	Pos	0.95
2	Pos	0.86
3	Pos	0.69
4	Neg	0.65
5	Pos	0.59
6	Neg	0.52
7	Pos	0.51
8	Neg	0.39
9	Neg	0.28
10	Neg	0.18
11	Pos	0.15
12	Neg	0.06



$$c = 0.3$$

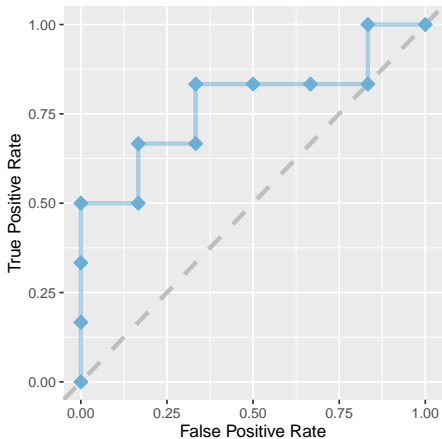
$$\rightarrow \text{TPR} = 0.833$$

$$\rightarrow \text{FPR} = 0.5$$

add plot showing sliding thresholds (suggestion Ludwig)

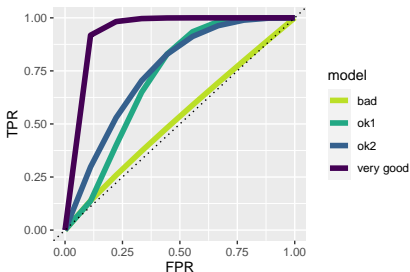
DRAWING ROC CURVES

#	Truth	Score
1	Pos	0.95
2	Pos	0.86
3	Pos	0.69
4	Neg	0.65
5	Pos	0.59
6	Neg	0.52
7	Pos	0.51
8	Neg	0.39
9	Neg	0.28
10	Neg	0.18
11	Pos	0.15
12	Neg	0.06



ROC CURVE PROPERTIES

- The closer the curve to the top-left corner, the better.
- If ROC curves cross, a different model might be better in different parts of the ROC space.



- Small thresholds will very liberally predict the positive class, and result in a potentially higher FPR, but also higher TPR.
- High thresholds will very conservatively predict the positive class, and result in a lower FPR and TPR.
- As we have not defined the trade-off between false positives and false negative costs, we cannot easily select the "best" threshold.
→ Visual inspection of all possible results seems useful.

AUC: AREA UNDER ROC CURVE

- $AUC \in [0, 1]$ is a single metric to evaluate scoring classifiers – independent of the chosen threshold.
 - $AUC = 1$: perfect classifier
 - $AUC = 0.5$: random, non-discriminant classifier
 - $AUC = 0$: perfect, with inverted labels
- The AUC is directly related to the Gini coefficient G :
 $AUC = 0.5 \cdot (G + 1)$. @BB: [check if correct/helpful here](#)

