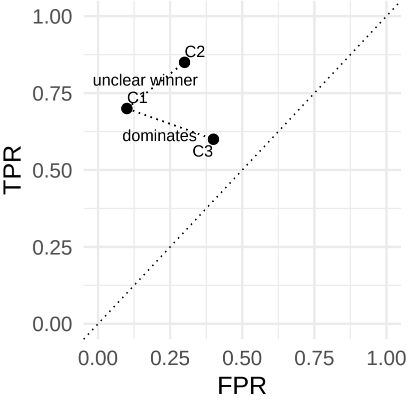
Introduction to Machine Learning

Evaluation: Measures for Binary Classification: ROC visualization

compstat-lmu.github.io/lecture_i2ml

LABELS: ROC SPACE

Plot True Positive Rate and False Positive Rate:



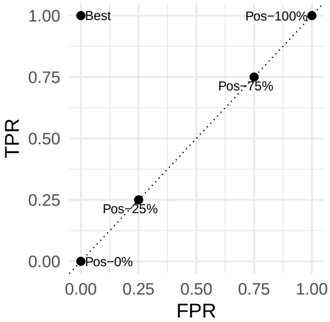
		True Class y	
		$+$	$-$
Pred.	$+$	TP	FP
$\hat{y}$	$-$	FN	TN

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

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

LABELS: ROC SPACE

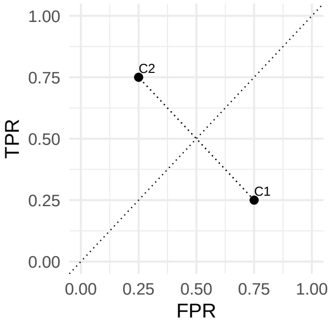
- The best classifier lies on the top-left corner
- The diagonal $\approx$ random labels (with different proportions).
  Assign positive *x* as "pos" with 25% probability $\rightarrow$ $TPR = 0.25$.
  Assign negative *x* as "pos" with 25% probability $\rightarrow$ $FPR = 0.25$.



LABELS: ROC SPACE

In practice, we should never obtain a classifier below the diagonal.

Inverting the predicted labels ($0 \rightarrow 1$ and $1 \rightarrow 0$) will result in a reflection at the diagonal.



LABEL DISTRIBUTION IN TPR AND FPR

TPR and FPR are insensitive to the class distribution:
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

MCE = 35/100
$TPR = 0.8$
$FPR = 0.5$

Example 2:
Proportion $n_+/n_- = 2$

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

MCE = 45/150 = 30/100
$TPR = 0.8$
$FPR = 0.5$

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

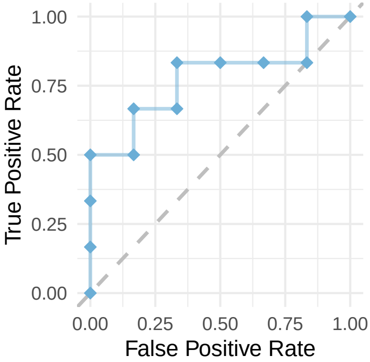
FROM PROBABILITIES TO LABELS: ROC CURVE

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

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

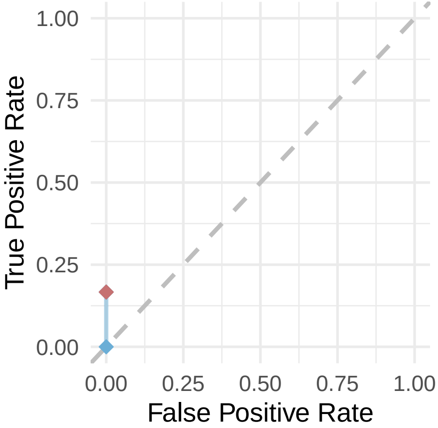
To draw a ROC curve: Iterate through all possible thresholds c

$\rightarrow$ Visual inspection of all possible thresholds / results



ROC CURVE

#	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



$c = 0.9$

$\rightarrow$ TPR = 0.167

$\rightarrow$ FPR = 0

ROC CURVE

#	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
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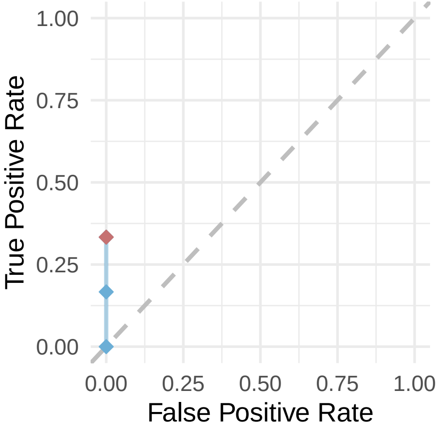


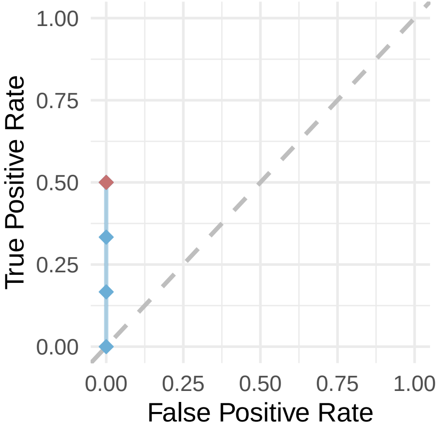
$c = 0.85$

$\rightarrow$ TPR = 0.333

$\rightarrow$ FPR = 0

ROC CURVE

#	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



$c = 0.66$
$\rightarrow$ TPR = 0.5
$\rightarrow$ FPR = 0

ROC CURVE

#	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
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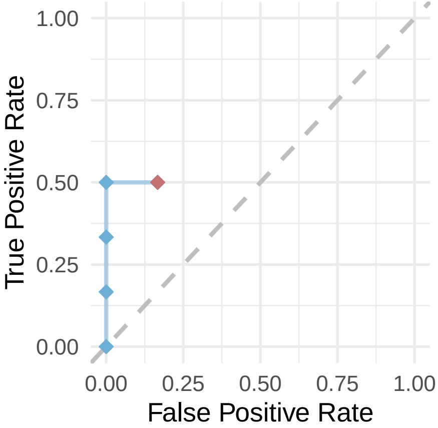
12	Neg	0.06



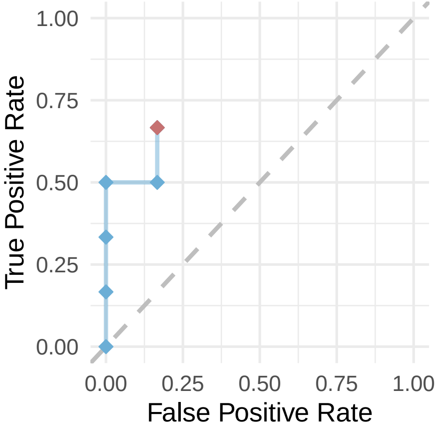
$c = 0.6$

$\rightarrow$ TPR = 0.5

$\rightarrow$ FPR = 0.167

ROC CURVE

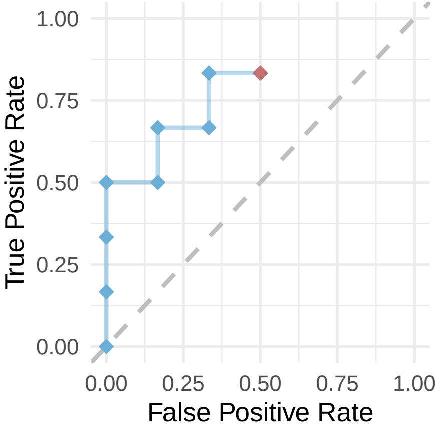
#	Truth	Score
1	Pos	0.95
2	Pos	0.86
3	Pos	0.69
4	Neg	0.65
5	Pos	0.59
6	Neg	0.52
7	Pos	0.51
8	Neg	0.39
9	Neg	0.28
10	Neg	0.18
11	Pos	0.15
12	Neg	0.06



$c = 0.55$
$\rightarrow$ TPR = 0.667
$\rightarrow$ FPR = 0.167

ROC CURVE

#	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



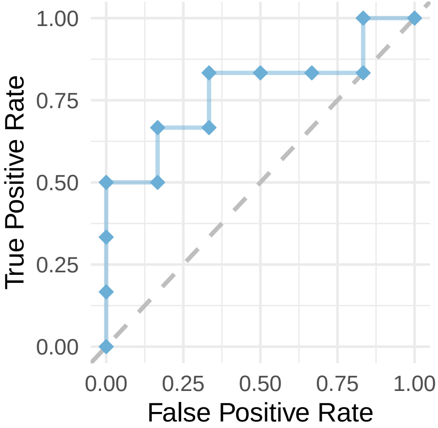
$c = 0.3$

$\rightarrow$ TPR = 0.833

$\rightarrow$ FPR = 0.5

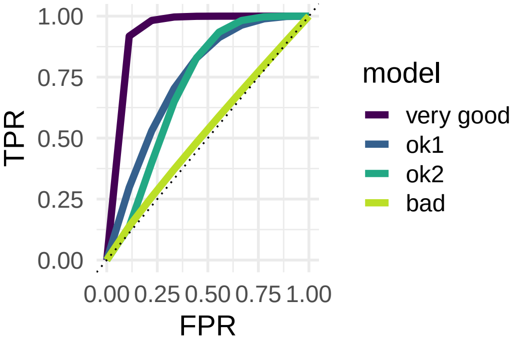
ROC CURVE

#	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



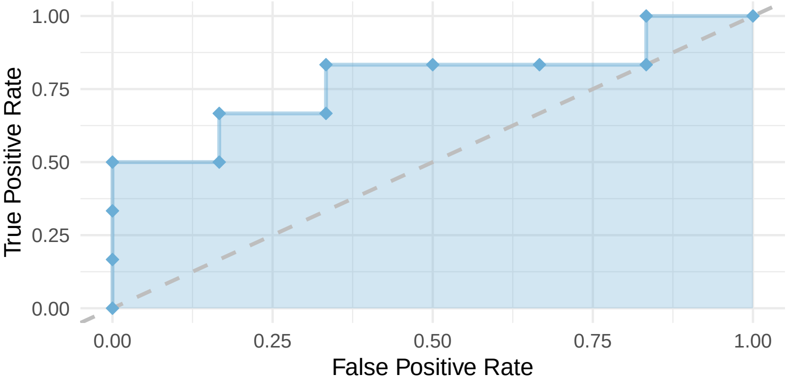
ROC CURVE

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



AUC: AREA UNDER ROC CURVE

- The AUC (in [0,1]) is a single metric to evaluate scoring classifiers
- AUC = 1: Perfect classifier
- AUC = 0.5: Randomly ordered



AUC: AREA UNDER ROC CURVE

Interpretation: Probability that classifier ranks a random positive higher than a random negative observation

Truth	Score
1	0.9
1	0.76
1	0.7
0	0.5
1	0.45
0	0.3
0	0.1

Choose a random positive

1	0.76

Choose a random negative

0	0.3

AUC = 0.9167

Classifier ranks the positive higher than the negative (with probability 0.9167)

PARTIAL AUC

- Sometimes it can be useful to look at a specific region under the ROC curve ⇒ partial AUC (pAUC).
- Examples: focus on a region with low FPR or a region with high TPR: