Evaluation Metrics
CS229

Nandita Bhaskhar
(Adapted from past CS229 teams)

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Topics

- Why are metrics important?
- Binary classifiers
  - Rank view, Thresholding
- Metrics
  - Confusion Matrix
  - Point metrics: Accuracy, Precision, Recall / Sensitivity, Specificity, F-score
  - Summary metrics: AU-ROC, AU-PRC, Log-loss.
- Class Imbalance
  - Failure scenarios for each metric
- Multi-class
- Choosing Metrics
- Unsupervised, Regression, Segmentation Metrics

Why are metrics important?

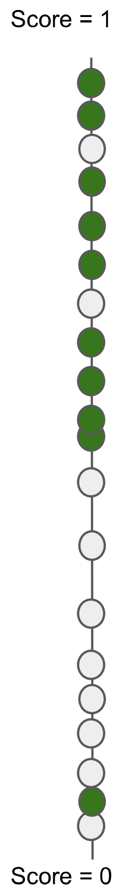
- Training objective (cost function) is only a proxy for real world objectives.
- Metrics help capture a business goal into a quantitative target (not all errors are equal).
- Helps organize ML team effort towards that target.
    - Generally in the form of improving that metric on the dev set.
- Useful to quantify the “gap” between:
    - Desired performance and baseline (estimate effort initially).
    - Desired performance and current performance.
    - Measure progress over time.
- Useful for lower level tasks and debugging (e.g. diagnosing bias vs variance).
- Ideally training objective should be the metric, but not always possible. Still, metrics are useful and important for evaluation.

Binary Classification

Binary Classification

- x is input
- y is binary output (0/1)
- Model is $\hat{y} = h(x)$
- Two types of models
  - Models that output a categorical class directly (K-nearest neighbor, Decision tree)
  - Models that output a real valued score (SVM, Logistic Regression)
    - Score could be margin (SVM), probability (LR, NN)
    - Need to pick a threshold
    - We focus on this type (the other type can be interpreted as an instance)

Score based models

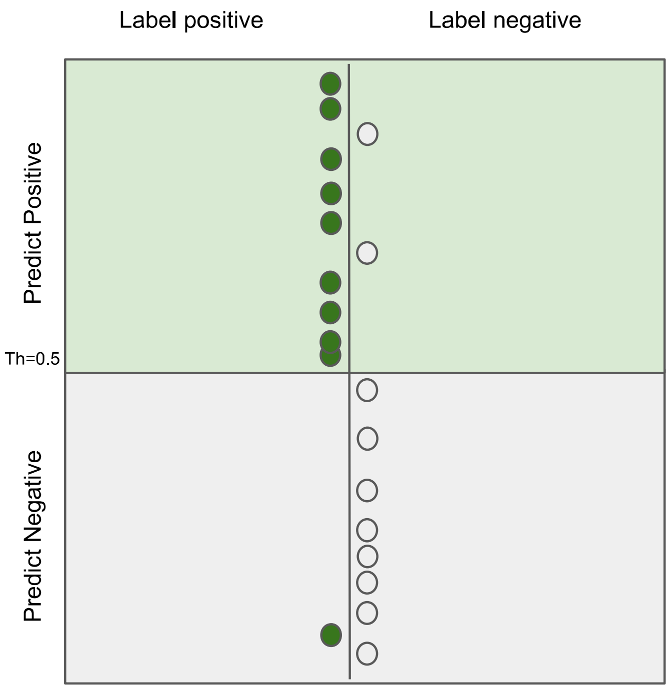


●	Positive example
○	Negative example

Example of Score: Output of logistic regression.
For most metrics: Only ranking matters.
If too many examples: Plot class-wise histogram.

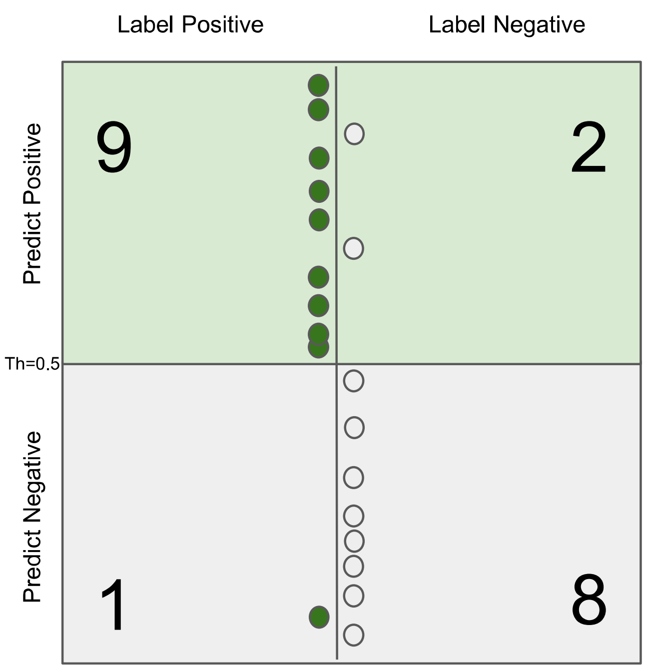
$$\text{Prevalence} = \frac{\text{\# positive examples}}{\text{\# positive examples} + \text{\# negatives examples}}$$

Threshold → Classifier → Point Metrics



Th
0.5

Point metrics: Confusion Matrix



Th
0.5

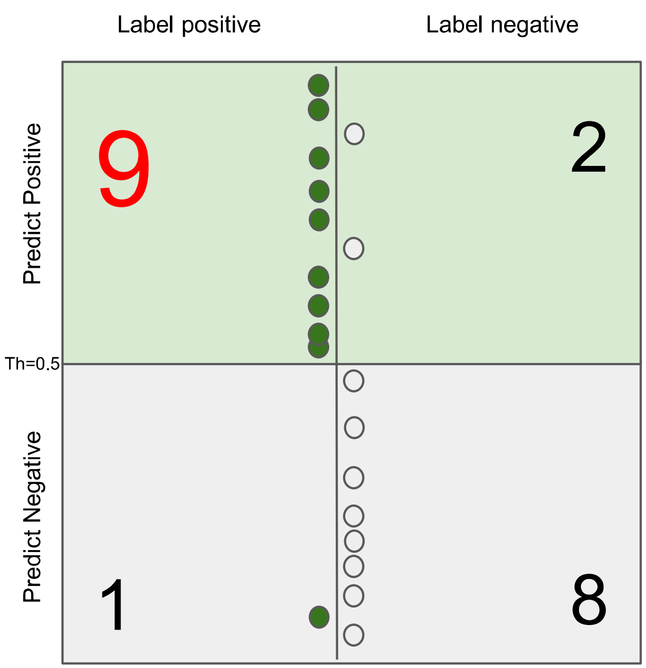
Properties:

- Total sum is fixed (population).
- Column sums are fixed (class-wise population).
- Quality of model & threshold decide how columns are split into rows.
- We want diagonals to be “heavy”, off diagonals to be “light”.

Source: Wikipedia

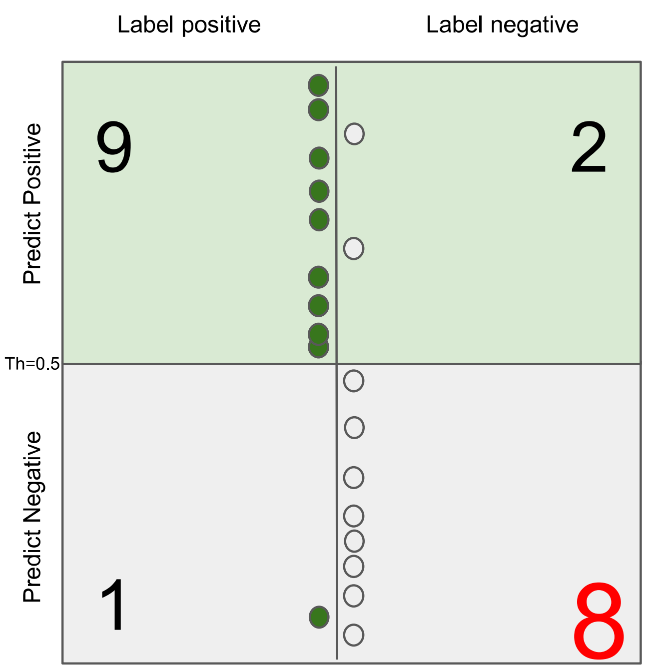
		Predicted condition			
	Total population $= P + N$	**Positive (PP)**	**Negative (PN)**	Informedness, bookmaker informedness (BM) $= TPR + TNR - 1$	Prevalence threshold (PT) $= \frac{\sqrt{TPR \times FPR} - FPR}{TPR - FPR}$
Actual condition	**Positive (P)**	**True positive (TP),** hit	**False negative (FN),** type II error, miss, underestimation	True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power $= \frac{TP}{P} = 1 - FNR$	False negative rate (FNR), miss rate $= \frac{FN}{P} = 1 - TPR$
	Negative (N)	**False positive (FP),** type I error, false alarm, overestimation	**True negative (TN),** correct rejection	False positive rate (FPR), probability of false alarm, fall-out $= \frac{FP}{N} = 1 - TNR$	True negative rate (TNR), specificity (SPC), selectivity $= \frac{TN}{N} = 1 - FPR$
	Prevalence $= \frac{P}{P + N}$	Positive predictive value (PPV), precision $= \frac{TP}{PP} = 1 - FDR$	False omission rate (FOR) $= \frac{FN}{PN} = 1 - NPV$	Positive likelihood ratio (LR+) $= \frac{TPR}{FPR}$	Negative likelihood ratio (LR−) $= \frac{FNR}{TNR}$
	Accuracy (ACC) $= \frac{TP + TN}{P + N}$	False discovery rate (FDR) $= \frac{FP}{PP} = 1 - PPV$	Negative predictive value (NPV) $= \frac{TN}{PN} = 1 - FOR$	Markedness (MK), deltaP (Δp) $= PPV + NPV - 1$	Diagnostic odds ratio (DOR) $= \frac{LR+}{LR-}$
	Balanced accuracy (BA) $= \frac{TPR + TNR}{2}$	F_1 score $= \frac{2 PPV \times TPR}{PPV + TPR} = \frac{2TP}{2TP + FP + FN}$	Fowlkes–Mallows index (FM) $= \sqrt{PPV \times TPR}$	Matthews correlation coefficient (MCC) $= \sqrt{TPR \times TNR \times PPV \times NPV} - \sqrt{FNR \times FPR \times FOR \times FDR}$	Threat score (TS), critical success index (CSI), Jaccard index $= \frac{TP}{TP + FN + FP}$

Point metrics: True Positives



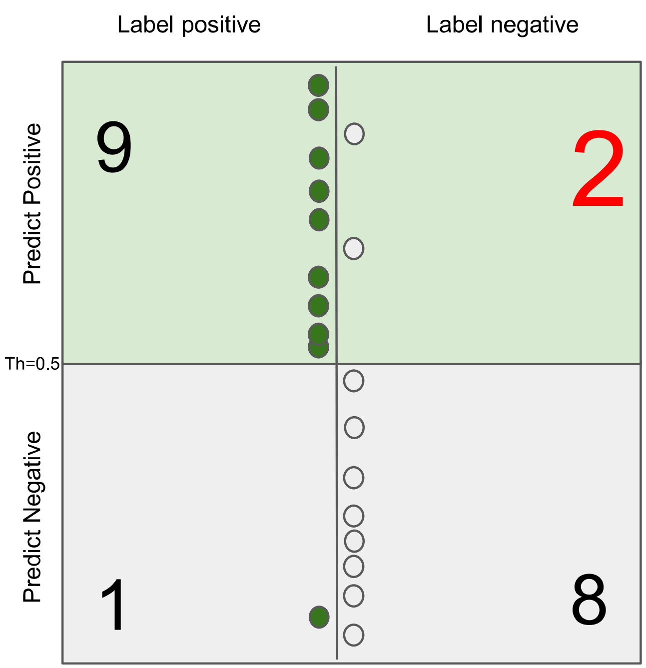
Th	TP
0.5	9

Point metrics: True Negatives



Th	TP	TN
0.5	9	8

Point metrics: False Positives

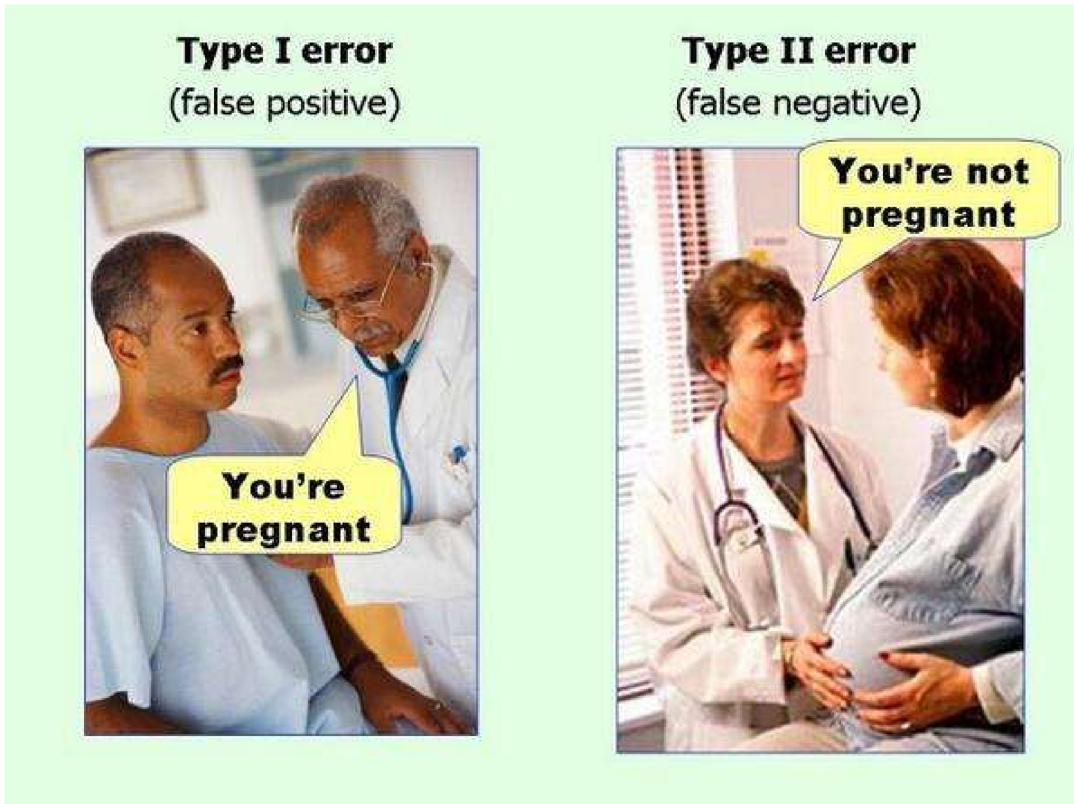


Th	TP	TN	FP
0.5	9	8	2

Point metrics: False Negatives

Th	TP	TN	FP	FN
0.5	9	8	2	1

FP and FN also called Type-1 and Type-2 errors



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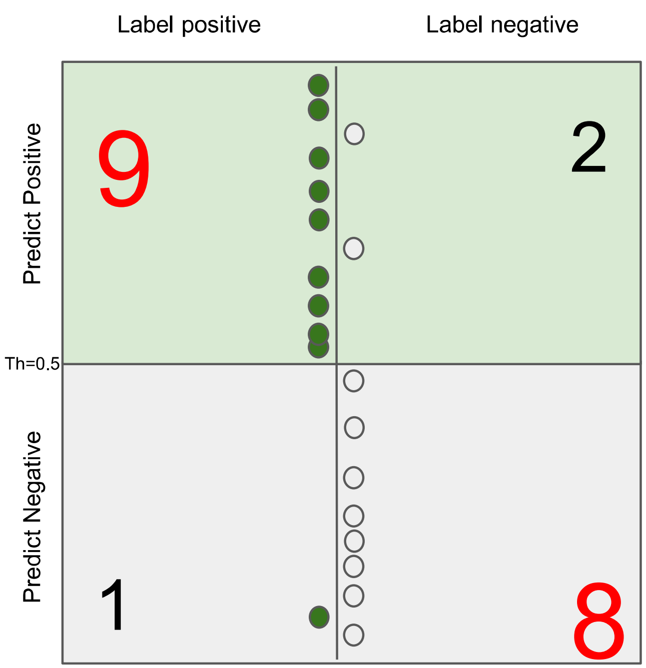
Point metrics: Accuracy



Th	TP	TN	FP	FN	Acc
0.5	9	8	2	1	0.85

Equivalent to 0-1 Loss!

Source: Wikipedia

		Predicted condition			
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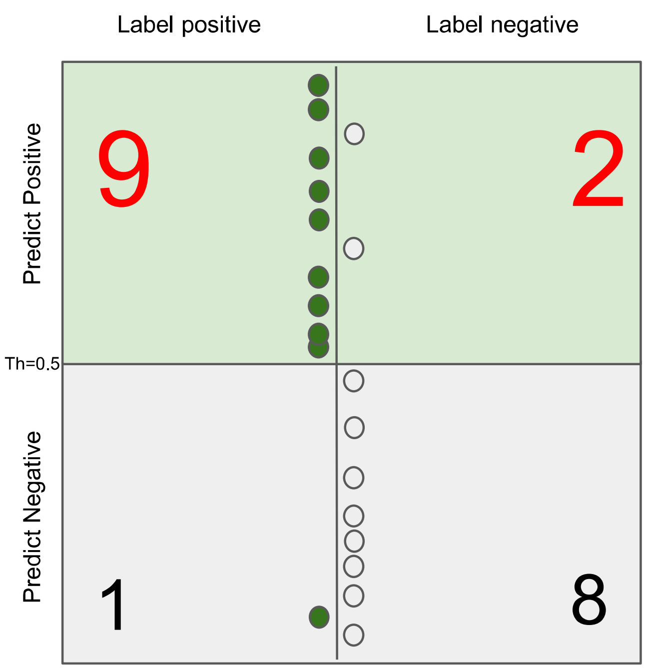
Point metrics: Precision



Th	TP	TN	FP	FN	Acc	Prec
0.5	9	8	2	1	0.85	0.81

Source: Wikipedia

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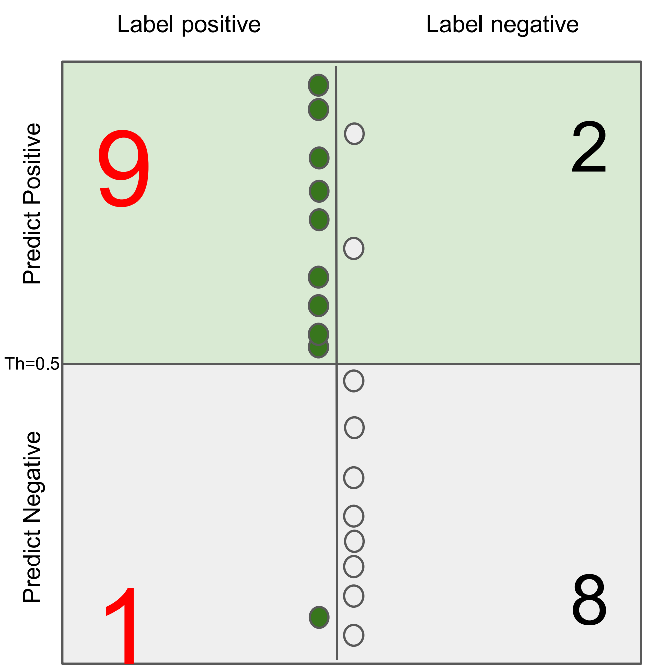
Point metrics: Positive Recall (Sensitivity)



Th	TP	TN	FP	FN	Acc	Prec	Recall
0.5	9	8	2	1	0.85	0.81	0.90

Source: Wikipedia

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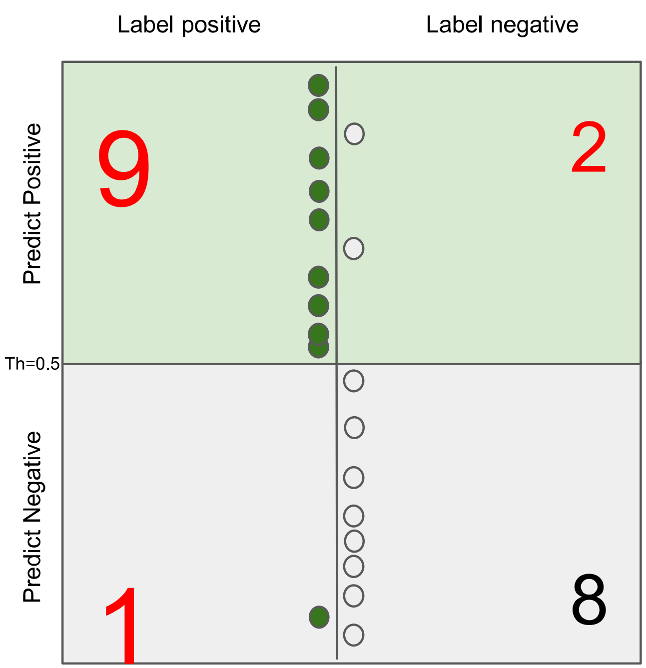
Point metrics: Precision vs Recall



Th	TP	TN	FP	FN	Acc	Prec	Recall
0.5	9	8	2	1	0.85	0.81	0.90

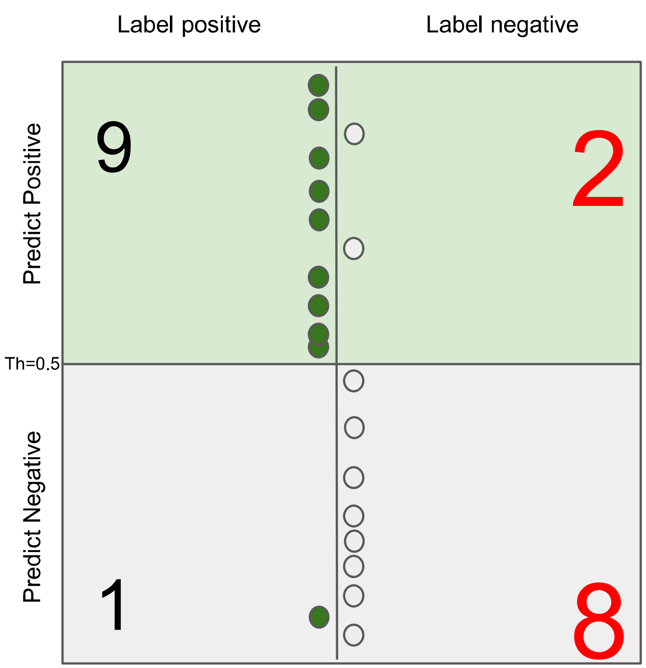
Trivial 100% recall?
Pull everybody above the threshold.

Trivial 100% precision?
Push everybody below the threshold except 1 green on top. (Hopefully no gray above it!)

Striving for good precision with 100% recall =
pulling up the lowest green as high as possible in the ranking.

Striving for good recall with 100% precision =
pushing down the top gray as low as possible in the ranking.

Point metrics: Negative Recall (Specificity)



Th	TP	TN	FP	FN	Acc	Prec	Recall
0.5	9	8	2	1	0.85	0.81	0.90

Sens.	Spec.
0.90	0.80

Source: Wikipedia

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Point metrics: F1-score

Th	TP	TN	FP	FN	Acc	Prec	Recall	Sens.	Spec.	F1
0.5	9	8	2	1	0.85	0.81	0.90	0.90	0.80	0.857

$$F_1 = \left(\frac{2}{\mathrm{recall}^{-1} + \mathrm{precision}^{-1}}\right) = 2 \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}.$$

Source: Wikipedia

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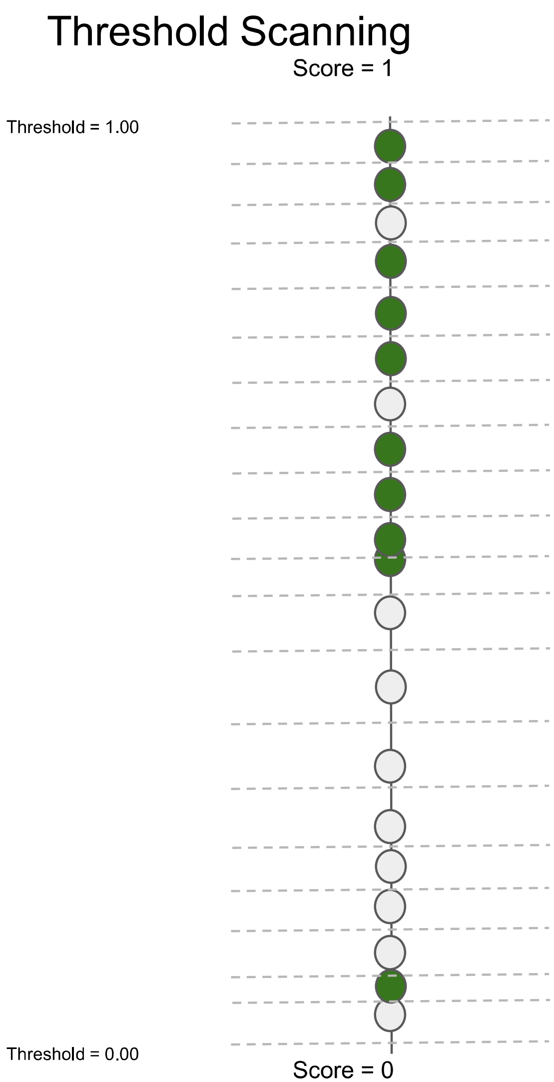
Point metrics: Changing threshold

Th	TP	TN	FP	FN	Acc	Prec	Recall	F1
0.6	7	8	2	3	0.75	0.77	0.70	0.733

Sens.	Spec.
0.70	0.80

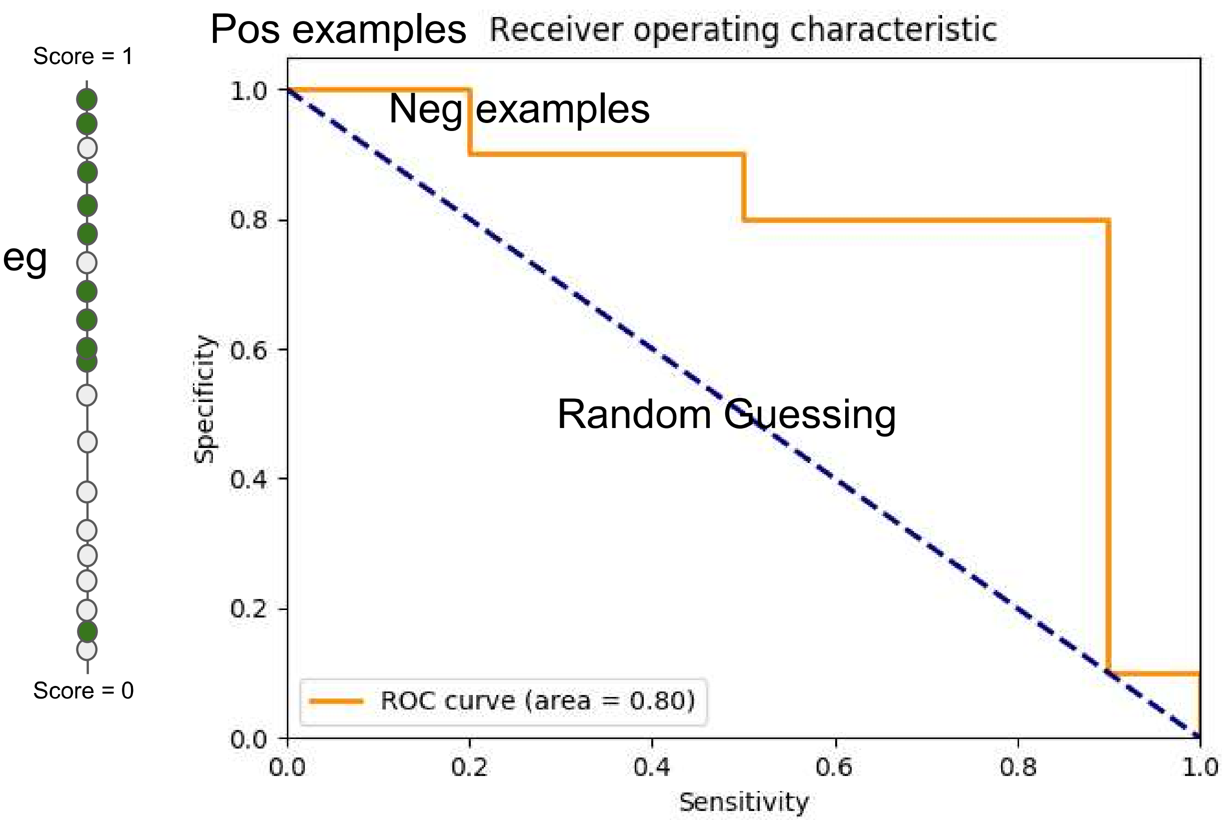
effective thresholds = # examples + 1



Threshold	TP	TN	FP	FN	Accuracy	Precision	Recall	Specificity	F1
1.00	0	10	0	10	0.50	1	0	1	0
0.95	1	10	0	9	0.55	1	0.1	1	0.182
0.90	2	10	0	8	0.60	1	0.2	1	0.333
0.85	2	9	1	8	0.55	0.667	0.2	0.9	0.308
0.80	3	9	1	7	0.60	0.750	0.3	0.9	0.429
0.75	4	9	1	6	0.65	0.800	0.4	0.9	0.533
0.70	5	9	1	5	0.70	0.833	0.5	0.9	0.625
0.65	5	8	2	5	0.65	0.714	0.5	0.8	0.588
0.60	6	8	2	4	0.70	0.750	0.6	0.8	0.667
0.55	7	8	2	3	0.75	0.778	0.7	0.8	0.737
0.50	8	8	2	2	0.80	0.800	0.8	0.8	0.800
0.45	9	8	2	1	0.85	0.818	0.9	0.8	0.857
0.40	9	7	3	1	0.80	0.750	0.9	0.7	0.818
0.35	9	6	4	1	0.75	0.692	0.9	0.6	0.783
0.30	9	5	5	1	0.70	0.643	0.9	0.5	0.750
0.25	9	4	6	1	0.65	0.600	0.9	0.4	0.720
0.20	9	3	7	1	0.60	0.562	0.9	0.3	0.692
0.15	9	2	8	1	0.55	0.529	0.9	0.2	0.667
0.10	9	1	9	1	0.50	0.500	0.9	0.1	0.643
0.05	10	1	9	0	0.55	0.526	1	0.1	0.690
0.00	10	0	10	0	0.50	0.500	1	0	0.667

Summary metrics: Rotated ROC (Sen vs. Spec)

Specificity
= True Neg / Neg



AUROC = Area Under ROC

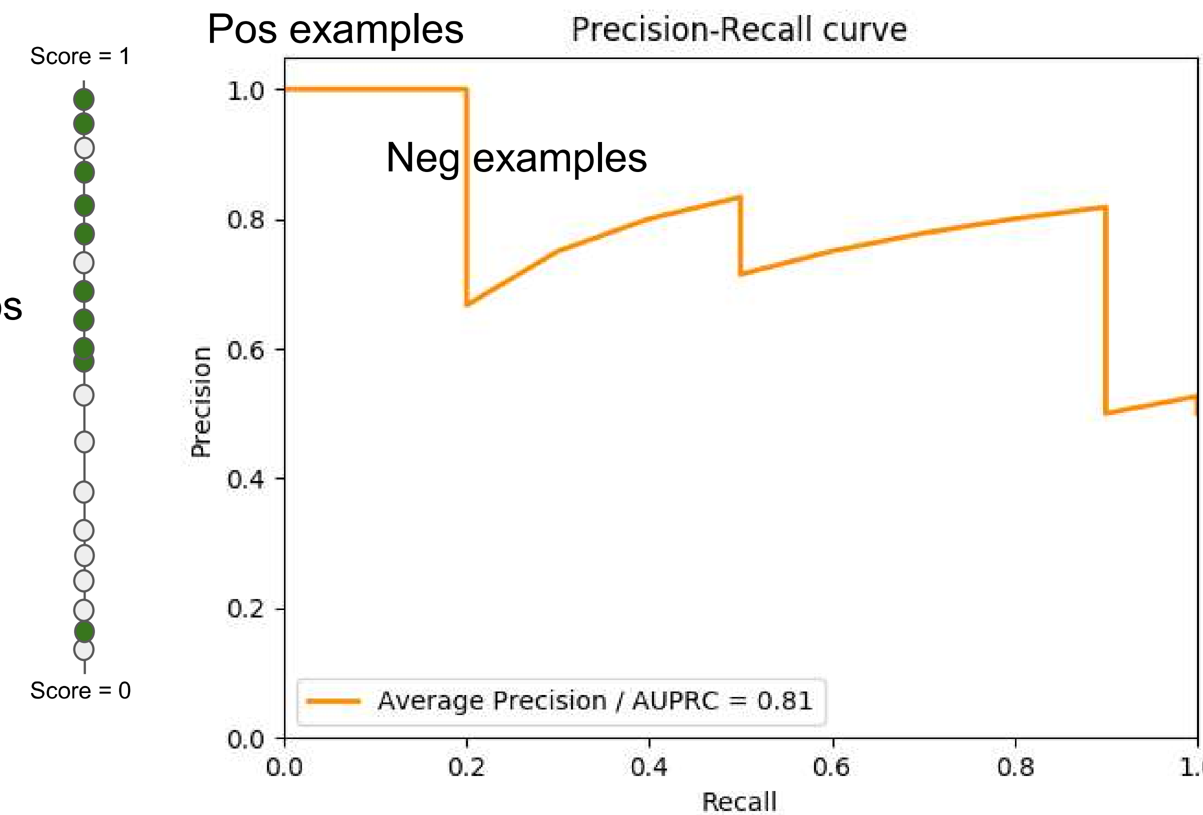
= Prob[Random Pos ranked higher than random Neg]

Agnostic to prevalence!

Sensitivity = True Pos / Pos

Summary metrics: PRC (Recall vs. Precision)

Precision
= True Pos /
Predicted Pos



AUPRC = Area Under PRC

= Expected precision for
Random threshold

When threshold = 0:
Precision = prevalence

Recall = Sensitivity = True Pos / Pos

Summary metrics:

Two models scoring the same data set. Is one of them better than the other?

Summary metrics: Log-Loss vs Brier Score

- Same ranking, and therefore the same AUROC, AUPRC, accuracy!

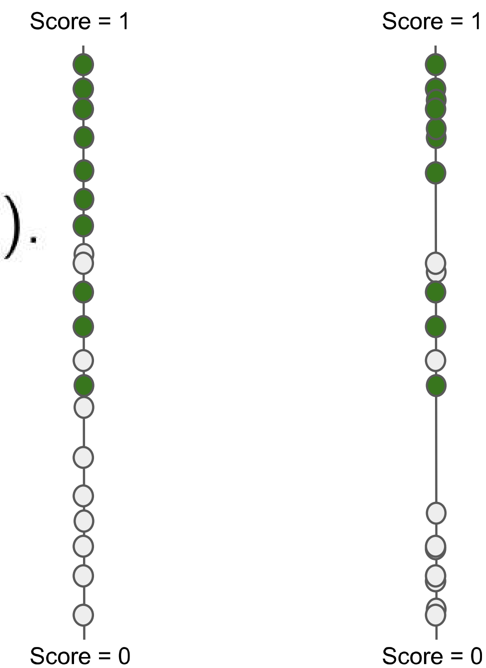
$$\text{Log Loss} = \frac{1}{N}\sum_{i=1}^{N} -y_i \log \hat{y}_i - (1 - y_i)\log(1 - \hat{y}_i).$$

- Rewards confident correct answers, heavily penalizes confident wrong answers.
- One perfectly confident wrong prediction is fatal.

-> Well-**calibrated** model

- **Proper** scoring rule: Minimized at $\hat{y} = y$

$$\text{Brier Score} = \frac{1}{N}\sum_{i=1}^{N} (\hat{y}_i - y_i)^2$$



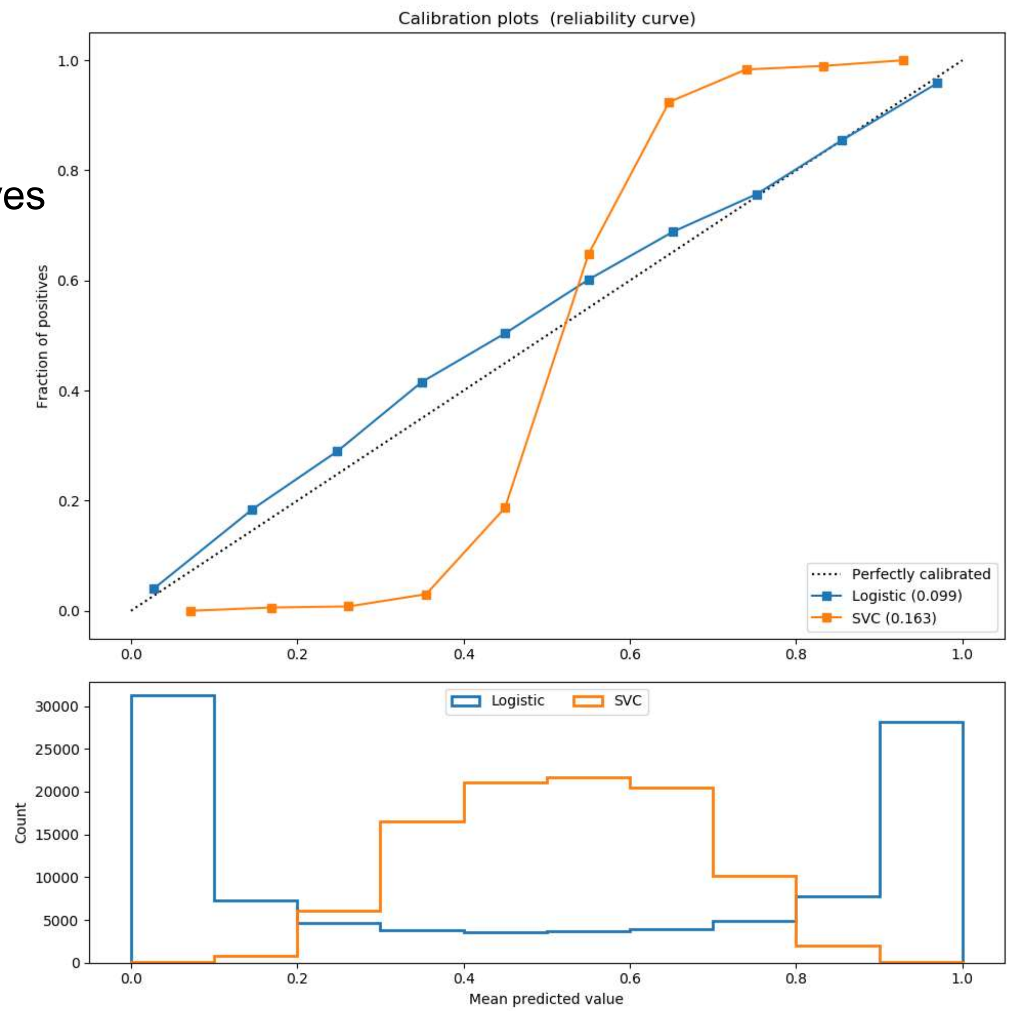
Calibration vs Discriminative Power

Logistic (th=0.5):
  Precision: 0.872
  Recall: 0.851
  F1: 0.862
  Brier: 0.099

SVC (th=0.5):
  Precision: 0.872
  Recall: 0.852
  F1: 0.862
  Brier: 0.163

Fraction of Positives

Histogram



Output

Binary Classification Under Class Imbalance

Class Imbalance

Symptom: Prevalence < 5% (no strict definition)

Metrics: May not be meaningful.

Learning: May not focus on minority class examples at all

(majority class can overwhelm logistic regression, to a lesser extent SVM)

What happen to the metrics under class imbalance?

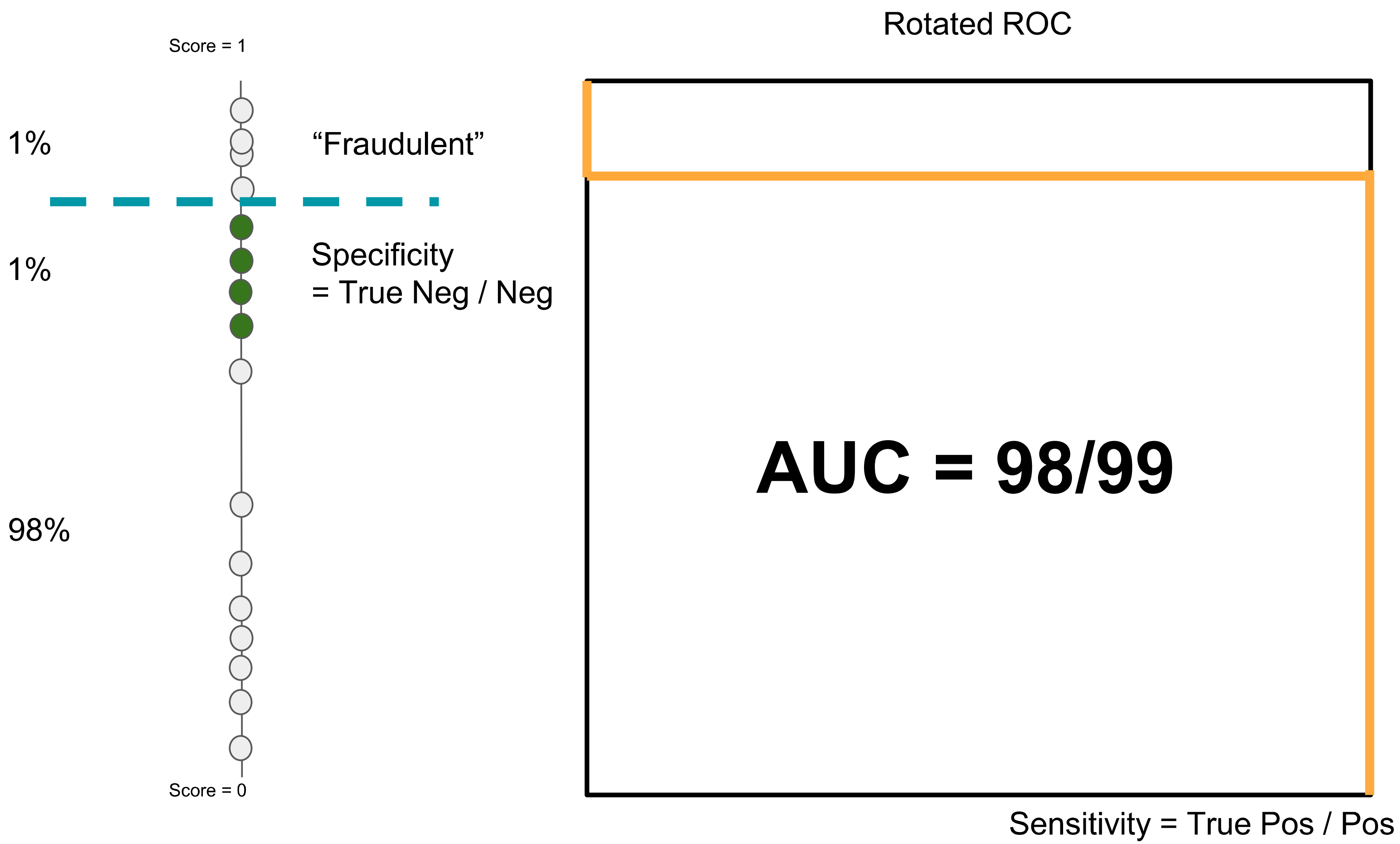
Accuracy: Blindly predicts majority class -> prevalence is the baseline.

Log-Loss: Majority class can dominate the loss.

AUROC: Easy to keep AUC high by scoring most negatives very low.

AUPRC: More robust than AUROC. But other challenges.

In general: Accuracy < AUROC < AUPRC


Score = 1
1%
"Fraudulent"
1%
Specificity
= True Neg / Neg
98%
Score = 0
Rotated ROC
AUC = 98/99
Sensitivity = True Pos / Pos

Multi-Class Classification

Multi-class

(white board)

- Confusion matrix will be N * N (still want heavy diagonals, light off-diagonals)
- Most metrics (except accuracy) generally analyzed as multiple 1-vs-many
- Multiclass variants of other metrics (micro vs macro averaging)
  - Macro: Class-wise, each class is given the same weightage
  - Micro: No class differences considered. F1 = Pr = Re = Acc
- Class imbalance is common (both in absolute and relative sense)
- Cost sensitive learning techniques (also helps in binary Imbalance)
  - Assign weights for each block in the confusion matrix.
  - Incorporate weights into the loss function.

Choosing Metrics

Choosing Metrics

Some common patterns:

- High precision is hard constraint, do best recall (search engine results, grammar correction): Intolerant to FP
  - Metric: Recall at Precision = XX %
- High recall is hard constraint, do best precision (medical diagnosis): Intolerant to FN
  - Metric: Precision at Recall = 100 %
- Capacity constrained (by K)
  - Metric: Precision in top-K.
- ……

Unsupervised Learning, Regression, Semantic Segmentation

Unsupervised Learning

- Log P(x) is a measure of fit in Probabilistic models (GMM, Factor Analysis)
    - High log P(x) on training set, but low log P(x) on test set is a measure of overfitting
    - Raw value of log P(x) hard to interpret in isolation

- K-means is trickier (because of fixed covariance assumption)

Regression

Common metrics:

- MSE: penalizes larger errors more
- MAE: penalizes all errors equally
- (others: Max Error, Mean squared logarithmic error, Mean absolute percentage error, Median absolute error, Pinball loss, …)

Semantic Segmentation

- Binary Mask prediction: so all binary classification metrics hold

But more important:

- DICE Score: Dice Sørensen Coefficient
  - Equivalent to F1 Score
  - $\frac{2\ |A \cap B|}{|A|+|B|}$

- IoU / Jaccard Metric

Thank You!