Data

Data Science Example

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After a few days, you have trained a model that predicts numbers resembling the ones in the table.

You contact the medical researcher and discuss the results.

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Researcher: Well, first, there is field 5, the variable we want to predict. It's common knowledge among people who analyze this type of data that results are better if you work with the log of the values, but I didn't discover this until later. Was it mentioned to you?

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Data Miner: No.

Model Dicsuccion

Researcher: But surely you heard about what happened to field 4? It's supposed to be measured on a scale from 1 to 10, with 0 indicating a missing value, but because of a data entry error, all 10's were changed into 0's. Unfortunately, since some of the patients have missing values for this field, it's impossible to say whether a 0 in this field is a real 0 or a 10. Quite a few of the records have that problem.

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Data Miner: Interesting. Were there any other problems?
Researcher: Yes, fields 2 and 3 are basically the same, but I assume that you probably noticed that.
Data Miner: Yes, but these fields were only weak predictors of field 5.

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Researcher: Anyway, given all those problems, I'm surprised you were able to accomplish anything.
Data Miner: True, but my results are really quite good. Field 1 is a very strong predictor of field 5. I'm surprised that this wasn't noticed before.
Researcher: What? Field 1 is just an identification number.
Data Miner: Nonetheless, my results speak for themselves.
Researcher: Oh, no! I just remembered. We assigned ID numbers after we sorted the records based on field 5. There is a strong connection, but it isn't very sensible. Sorry.

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OK, what's the point?

You have to

Understand the task you want to solve and the data!

Data Objects

Data objects represent entities we work with (e.g., classify them).

For example, in cancer prediction, the data objects are patients. In fruit classification, the data objects are individual fruits.

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Data objects are described by *attributes* (or *features* or *variables*).

For example, the age, weight, genetic profile, and other patient characteristics. Or the width and height of a fruit.

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One may make some distinctions

- *Attributes* represent information about the object without any additional assumptions.
- *Features* assume that their values are somewhat characteristic of the object.
- *Variables* assume that there is some process behind them (typically a random process in the case of statistics).

Data Types - Categorical Attributes

Categorical attributes (nominal attributes) are symbols or names of things.

- Each value represents some kind of category, code, or state.
- Values are not ordered and should not be used quantitatively (in computer science, the values are known as enumerations).

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- **Examples:**

$$\text{hair\_color} \in \{\text{black}, \text{brown}, \text{blond}, \text{red}, \text{auburn}, \text{gray}, \text{white}\}$$

$$\text{marital\_status} \in \{\text{single}, \text{married}, \text{divorced}, \text{widowed}\}$$

$$\text{customer\_ID} \in \{0, 1, 2, \ldots\}$$

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Binary attributes are categorical attributes with only two values.

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$$\text{drink\_size} \in \{\text{small}, \text{medium}, \text{large}\}$$

$$\text{grades} \in \{\text{A}, \text{B}, \text{C}, \text{D}, \text{E}, \text{F}\}$$

It can also be obtained by discretizing numeric quantities into series of intervals.

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Categorical and ordinal attributes are called *qualitative* attributes.

Next, we look at numeric, i.e., *quantitative* attributes.

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Distinguish two types: *Interval-scale* and *ratio-scale*.

	INTERVAL SCALE	**RATIO SCALE**
Measurement interval	Equal intervals between consecutive points.	Equal intervals with the presence of a true zero.
Absolute zero	Lacks a true zero point.	Possesses a true zero point.
Statistical analysis	Limited to addition and subtraction	Allows for meaningful multiplication and division.
Meaningful ratios	Ratios are not meaningful due to the lack of zero.	Ratios are meaningful due to the presence of zero.
Examples	IQ scores, Celsius temperature, NPS data, etc.	Height, weight, income, etc.

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- *Continuous*

  An uncountably infinite range of values, typically an interval.

  There are several more or less formal definitions of continuous attributes in the literature. For example:

  - All non-discrete variables.
  - Have an infinite number of values between any two values.
  - Their values are measured (??).

Deeper characteristics of data (statistical properties, etc.) will be examined at tutorials.

Classifier Evaluation

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There are many possible metrics ...

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I will call the class 1 *positive* and the class 0 *negative*.

Note that the class 0 is not negative in the numerical sense but in the absence of something (e.g., predicted illness).

Confusion Matrix for Binary Classifier

		Predicted	
		1	0
Actual	1	TP	FN
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Example

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Assume that we have trained a classifier with the following results:

Index	1	2	3	4	5	6	7	8	9	10	11	12
Actual	1	1	1	1	1	1	1	1	0	0	0	0
Predicted	0	0	1	1	1	1	1	1	1	0	0	0
Result	FN	FN	TP	TP	TP	TP	TP	TP	FP	TN	TN	TN

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Result	FN	FN	TP	TP	TP	TP	TP	TP	FP	TN	TN	TN

Actual condition	**Predicted condition**	
	Cancer	**Non-cancer**
Cancer	TP $=6$	FN $=2$
Non-cancer	FP $=1$	TN $=3$
Total	$8+4=12$	

Terminology

- TP aka hit
- TN aka correct rejection
- FP aka type I error, false alarm, overestimation
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In what follows, we also use

- $\mathrm{P} = \mathrm{TP} + \mathrm{FN}$ of all cases with the *actual* class 1
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- $\mathrm{PP} = \mathrm{TP} + \mathrm{FP}$ of all cases with the *predicted* class 1
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There is a large number of derived metrics. We consider some of the most used in practice.

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Actual condition	**Predicted condition**	
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The Accuracy is

$$\text{ACC} = \frac{\mathsf{TP} + \mathsf{TN}}{\mathsf{P} + \mathsf{N}} = \frac{6+3}{12} = \frac{3}{4}$$

Accuracy - Imbalanced Classes

Accuracy can be misleading when the classes are imbalanced:

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However, the classifier is pretty bad in the positive cases.

In the case of cancer prediction, such a classifier would be a disaster.

Precision & Recall

To mitigate the defect of the Accuracy, we may compute the following metrics:

$$\text{Precision} = \frac{\text{TP}}{\text{PP}} \quad (= \text{how often is predicted positive actually positive})$$

Precision is also known as positive predictive value (PPV)

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$$\text{Recall} = \frac{\mathsf{TP}}{\mathsf{P}} \quad (= \text{how often is actually positive predicted positive})$$

Recall is also known as true positive rate, sensitivity, hit rate, and power.

Precision & Recall - Example

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- Recall measures how often is an ill patient found to be ill (in our case, $6/8$)

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$$\text{Precision} = 1$$

$$\text{Recall} = \frac{1}{10}$$

You can see that the predictor is very precise (on the class 1) but useless due to the weak Recall.

Precision & Recall - Relative Importance

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Consider *Precision* and *Recall*.

By now, you should remember what they measure.

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Can we get a single number summarizing both Precision and Recall?

For example, to compare two classifiers.

F_1 Score

F_1 score is the harmonic mean of Recall and Precision:

$$\mathsf{F}_1 = \frac{2}{\mathsf{Recall}^{-1} + \mathsf{Precision}^{-1}} = \frac{2\mathsf{TP}}{2\mathsf{TP} + \mathsf{FP} + \mathsf{FN}}$$

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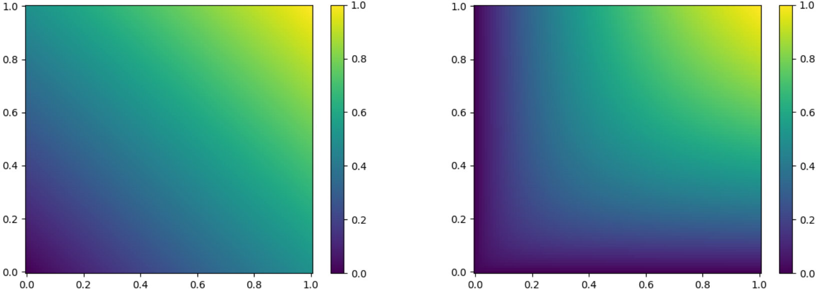
$$\mathrm{F}_1 = \frac{2}{\mathrm{Recall}^{-1} + \mathrm{Precision}^{-1}} = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

Compare the arithmetic (left) and harmonic (right) mean:



The harmonic mean prefers the two values closer to each other.

For example, the harmonic mean of $2/3$ and $1/3$ is (approx) 0.44444.

F_1 Score - Examples

Consider the cancer example:

Actual condition	**Predicted condition**	
	Cancer	**Non-cancer**
Cancer	TP = 6	FN = 2
Non-cancer	FP = 1	TN = 3
Total	8 + 4 = 12	

Here $F_1 = \frac{2\text{TP}}{2\text{TP}+\text{FP}+\text{FN}} = (2 \cdot 6)/((2 \cdot 6) + 1 + 2) = 0.8$.

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Our imbalanced example:

Actual	**Predicted**	
	Pos	**Neg**
Pos	1	9
Neg	0	90
Total	90 + 10 = 100	

Here $F_1 = \frac{2\mathrm{TP}}{2\mathrm{TP}+\mathrm{FP}+\mathrm{FN}} = (2 \cdot 1)/((2 \cdot 1) + 0 + 9) = 0.18.$

Note that the average of Precision and Recall is 0.55, which would give us a much less severe warning that the classifier is bad.

Imbalanced Classes Once More

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Consider

Actual	**Predicted**	
	Pos	**Neg**
Pos	90	0
Neg	9	1
Total	90 + 10 = 100	

$$\text{Precision} = 90/99 \qquad \text{Recall} = 90/90$$

$$F_1 = \frac{2\text{TP}}{2\text{TP} + \text{FP} + \text{FN}} = (2 \cdot 90)/(2 \cdot 90 + 9 + 0) = 0.95$$

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Actual	**Predicted**	
	Pos	**Neg**
Pos	90	0
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Total	$90 + 10 = 100$	

$$\text{Precision} = 90/99 \qquad \text{Recall} = 90/90$$

$$F_1 = \frac{2\text{TP}}{2\text{TP} + \text{FP} + \text{FN}} = (2 \cdot 90)/(2 \cdot 90 + 9 + 0) = 0.95$$

All great, except that the classifier sucks on the negative cases.

If you are concerned with the negative cases, swap the classes and compute another set of metrics.

F_1 Score

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- *Fowlkes-Mallows index* is a geometric mean of Precision and Recall (used in clustering).

  The geometric mean is between the arithmetic and harmonic mean. For example, the geometric mean of 2/3 and 1/3 is (approx) 0.4714.

More Derived Metrics

Positive predictive value (PPV), precision $= \frac{\mathrm{TP}}{\mathrm{PP}} = 1 - \mathrm{FDR}$	False omission rate (FOR) $= \frac{\mathrm{FN}}{\mathrm{PN}} = 1 - \mathrm{NPV}$
False discovery rate (FDR) $= \frac{\mathrm{FP}}{\mathrm{PP}} = 1 - \mathrm{PPV}$	Negative predictive value (NPV) $= \frac{\mathrm{TN}}{\mathrm{PN}} = 1 - \mathrm{FOR}$

You can see that the negative predictive value becomes the Precision when we swap the classes (and vice versa).

More Derived Metrics

True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power $= \frac{\mathrm{TP}}{\mathrm{P}} = 1 - \mathrm{FNR}$	False negative rate (FNR), miss rate $= \frac{\mathrm{FN}}{\mathrm{P}} = 1 - \mathrm{TPR}$
False positive rate (FPR), probability of false alarm, fall-out $= \frac{\mathrm{FP}}{\mathrm{N}} = 1 - \mathrm{TNR}$	True negative rate (TNR), specificity (SPC), selectivity $= \frac{\mathrm{TN}}{\mathrm{N}} = 1 - \mathrm{FPR}$

Note that *specificity* becomes Recall when we swap the classes (and vice versa).

For example, medical doctors communicate in terms of *sensitivity* and *specificity*.

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$$\text{TPR} = \text{Sensitivity} = \text{Recall} = \text{TP}/\text{P} = 6/8$$

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$$\text{FNR} = \text{Miss rate} = \text{FN}/\text{P} = 2/8$$

How often is positive predicted negative?

Evaluating Multi-class Classifiers

Classification Into Multiple Classes

Assume classification into classes from a finite set C.

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How good are the predictions $h_1, \ldots, h_p$ w.r.t. $c_1, \ldots, c_p$?

There are many possible metrics ...

Consider an arbitrary (finite) number of classes in C.

Confusion Matrix

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Formally,

$$M_{ij} = |\{k \mid c_k = i \wedge h_k = j\}|$$

Actual	**Predicted**				
	1	$\cdots$	j	$\cdots$	m
1	M_{11}	$\cdots$	M_{1j}	$\cdots$	M_{1m}
$\vdots$	$\vdots$		$\vdots$		$\vdots$
i	M_{i1}	$\cdots$	M_{ij}	$\cdots$	M_{im}
$\vdots$	$\vdots$		$\vdots$		$\vdots$
m	M_{m1}	$\cdots$	M_{mj}	$\cdots$	M_{mm}

Example

Actual	Predicted
big	big
big	big
small	big
medium	medium
big	small
big	big
small	small
small	small
medium	medium
medium	small
small	small
big	big
medium	small
small	medium

Example

Actual	Predicted
big	big
big	big
small	big
medium	medium
big	small
big	big
small	small
small	small
medium	medium
medium	small
small	small
big	big
medium	small
small	medium

Actual	**Predicted**		
	big	**medium**	**small**
big	5	0	1
medium	0	2	2
small	1	1	3

Note that the diagonal counts the correctly classified samples.

The off-diagonal elements correspond to misclassified samples.

Metrics

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$$\text{Precision}[i] = \frac{M_{ii}}{M_{\bullet i}} \qquad \text{Recall}[i] = \frac{M_{ii}}{M_{i\bullet}}$$

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$$\text{Precision}[i] = \frac{M_{ii}}{M_{\bullet i}} \qquad \text{Recall}[i] = \frac{M_{ii}}{M_{i\bullet}}$$

$$F_1[i] = \frac{2 * \text{Precision}[i] * \text{Recall}[i]}{\text{Precision}[i] + \text{Recall}[i]}$$

Note that Precision, Recall, and F_1 can be defined only for a given class!

Example

Actual	**Predicted**		
	big	**medium**	**small**
big	5	0	1
medium	0	2	2
small	1	1	3

Compute the metrics.

Example

$$\text{Accuracy} = (5+2+3)/15 = 0.66$$

$$\text{Precision[big]} = 5/6$$

$$\text{Precision[medium]} = 2/3$$

$$\text{Precision[small]} = 3/6$$

$$\text{Recall[big]} = 5/6$$

$$\text{Recall[medium]} = 2/4$$

$$\text{Recall[small]} = 3/5$$

Actual	**Predicted**		
	big	**medium**	**small**
big	5	0	1
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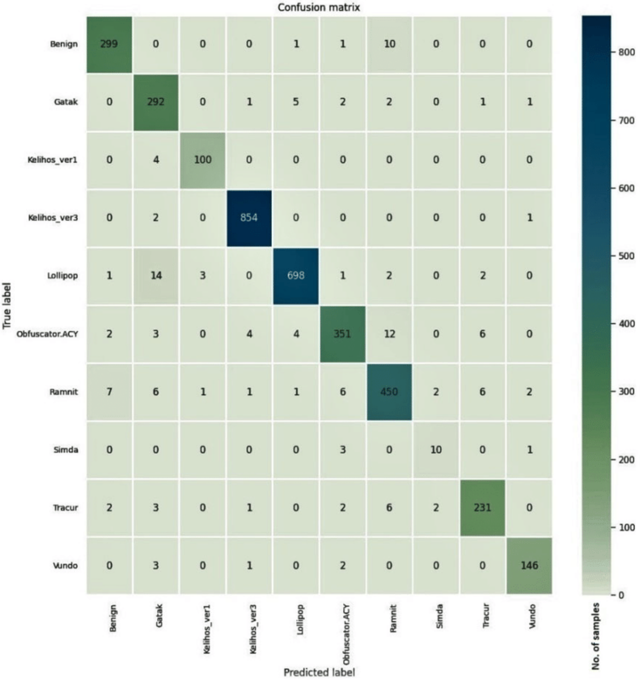
$$F_1[\text{big}] = \frac{2 * (5/6) * (5/6)}{(5/6) + (5/6)} = 5/6 = 0.83$$

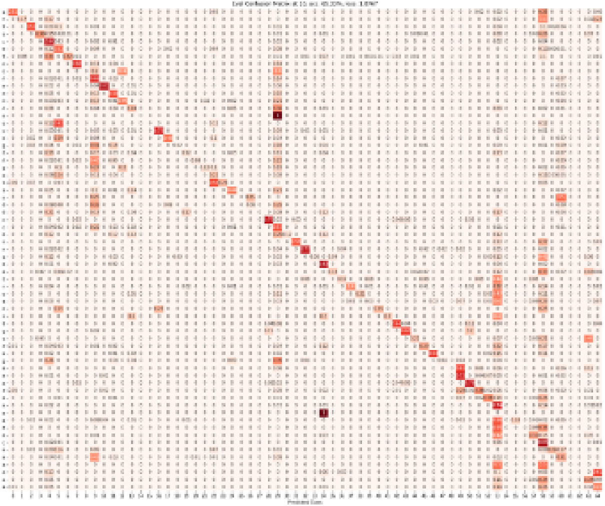
$$F_1[\text{medium}] = 0.57$$

$$F_1[\text{medium}] = 0.54$$

How do you get a single number out of these? Average Precision, Recall, and F_1 are usually computed, but one needs to be careful about the variance.



True label \ Predicted label	Benign	Gatak	Kelihos_ver1	Kelihos_ver3	Lollipop	Obfuscator.ACY	Ramnit	Simda	Tracur	Vundo
Benign	299	0	0	0	1	1	10	0	0	0
Gatak	0	292	0	1	5	2	2	0	1	1
Kelihos_ver1	0	4	100	0	0	0	0	0	0	0
Kelihos_ver3	0	2	0	854	0	0	0	0	0	1
Lollipop	1	14	3	0	698	1	2	0	2	0
Obfuscator.ACY	2	3	0	4	4	351	12	0	6	0
Ramnit	7	6	1	1	1	6	450	2	6	2
Simda	0	0	0	0	0	3	0	10	0	1
Tracur	2	3	0	1	0	2	6	2	231	0
Vundo	0	3	0	1	0	2	0	0	0	146



Machine learning/data mining is needed to understand the matrix.

Probabilistic Classifier Evaluation

Binary Probabilistic Classifier

Assume binary classification into two classes $\{0, 1\}$.

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Consider a sequence of predictions generated by a classifier.
Now the classifier returns *probability of class* 1 for a given input:

$$h_1, \ldots, h_p \in [0, 1]$$

Here each h_k has been predicted for the k-the example $(\vec{x}_k, c_k)$.

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Given a threshold $T \in [0, 1]$ we define

$$h_k^T = \begin{cases} 1 & \text{if } h_k \geq T \\ 0 & \text{if } h_k < T \end{cases}$$

For every T we can compute all the metrics (Precision, Recall, etc.)

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Given a metric MET and a threshold T, we denote by MET[T] the metric MET evaluated on $h_1^T, \ldots, h_p^T$.

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We obtain

$$\mathrm{TP}[T] = |\{k \mid h_k^T = 1 \wedge c_k = 1\}|$$

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and

$\text{TN}[T], \text{FP}[T], \text{FN}[T], \text{Accuracy}[T], \text{Precision}[T], \text{Recall}[T], F_1[T], \ldots$

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and
$\text{TN}[T], \text{FP}[T], \text{FN}[T], \text{Accuracy}[T], \text{Precision}[T], \text{Recall}[T], F_1[T], \dots$

However, all metrics are now functions of the threshold T.

Thresholded Classifier Metrics

Index	1	2	3	4	5	6	7	8	9	10	11	12
Actual	1	1	1	1	1	0	0	1	1	0	0	0
Predicted	.98	.95	.9	.86	.66	.48	.42	.4	.36	.15	.1	.05
T=0.5	TP	TP	TP	TP	TP	TN	TN	FN	FN	TN	TN	TN
T=0.42	TP	TP	TP	TP	TP	FP	FP	TP	FN	TN	TN	TN
T=0.1	TP	TP	TP	TP	TP	FP	FP	TP	TP	FP	FP	TN

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For example, consider $T = 0.42$, then

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T=0.1	TP	TP	TP	TP	TP	FP	FP	TP	TP	FP	FP	TN

For example, consider $T = 0.42$, then

$$\mathrm{TP}[T] = 6 \quad \mathrm{FP}[T] = 2 \quad \mathrm{FN}[T] = 1 \quad \mathrm{TN}[T] = 3$$

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For example, consider $T = 0.42$, then

$$\text{TP}[T] = 6 \quad \text{FP}[T] = 2 \quad \text{FN}[T] = 1 \quad \text{TN}[T] = 3$$

$$\text{Accuracy}[T] = \frac{3+6}{12} \quad \text{Precision}[T] = \frac{6}{6+2} \quad \text{Recall}[T] = \frac{5}{6+1}$$

Thresholded Classifier Metrics

Index	1	2	3	4	5	6	7	8	9	10	11	12
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T=0.1	TP	TP	TP	TP	TP	FP	FP	TP	TP	FP	FP	TN

For example, consider $T = 0.42$, then

$$\mathrm{TP}[T] = 6 \quad \mathrm{FP}[T] = 2 \quad \mathrm{FN}[T] = 1 \quad \mathrm{TN}[T] = 3$$

$$\mathrm{Accuracy}[T] = \frac{3+6}{12} \quad \mathrm{Precision}[T] = \frac{6}{6+2} \quad \mathrm{Recall}[T] = \frac{5}{6+1}$$

$$F_1[T] = \frac{2 \cdot 6/8 \cdot 5/7}{6/8 + 5/7} = 0.73$$

Receiver Operating Characteristic (ROC)

Consider two metrics for a given T:

$$\mathrm{TPR}[T] = \frac{\mathrm{TP}[\mathrm{T}]}{\mathrm{P}[T]} \qquad \text{(True Positive Rate)}$$

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$$\mathrm{ROC}(T) = (\mathrm{TPR}[T], \mathrm{FPR}[T])$$

Observe that

$$\mathrm{ROC}(0) = (1,1)$$

Because the classifier with $T = 0$ simply classifies everything as positive, i.e., into the class 1.

Both $\mathrm{TPR}[T]$ and $\mathrm{FPR}[T]$ are non-increasing in T.

Index	1	2	3	4	5	6	7	8	9	10	11	12
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ROC

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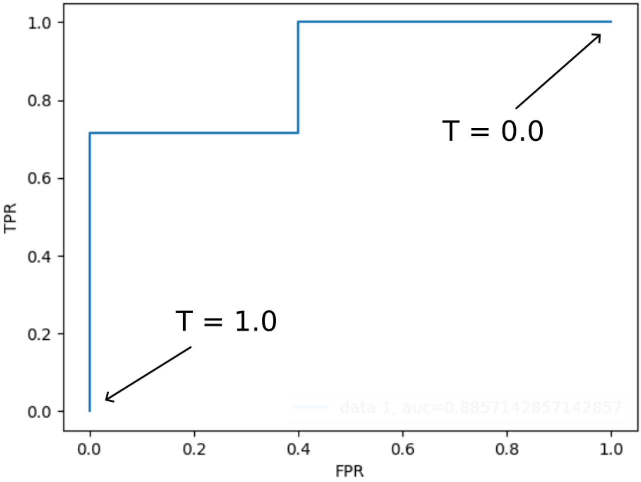
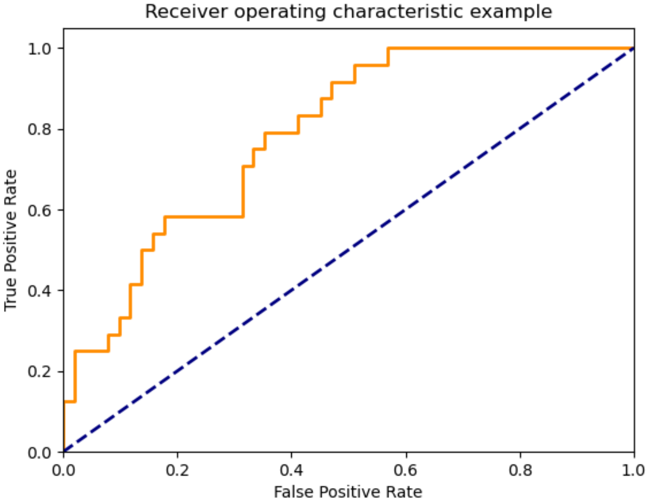
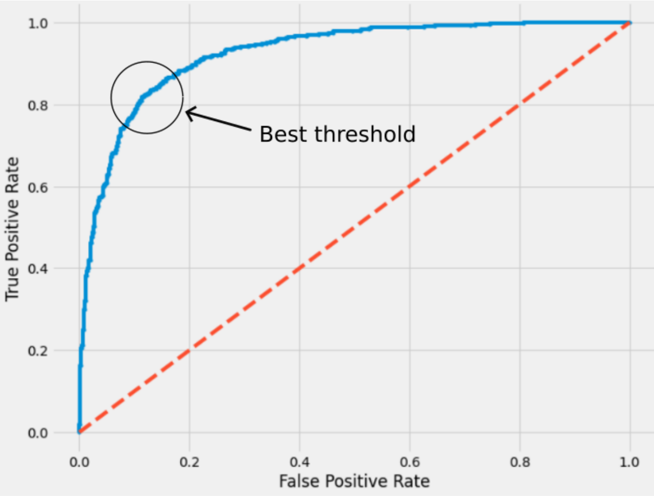


Iris Dataset - A Classifier



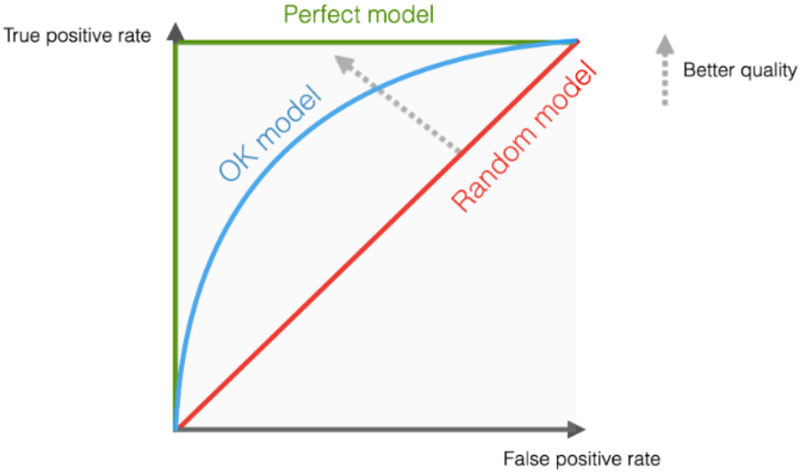
Example from the scikit-learn manual - SVM classifier trained in Iris

Using ROC and Threshold



Search for the best threshold at the elbow of the ROC curve.

ROC - Explanation



The larger the *area under the ROC curve (ROC-AUC)*, the better.

ROC-AUC ranges from 0 to 1. ROC-AUC ≈ 0.5 indicates random guessing.

ROC-AUC

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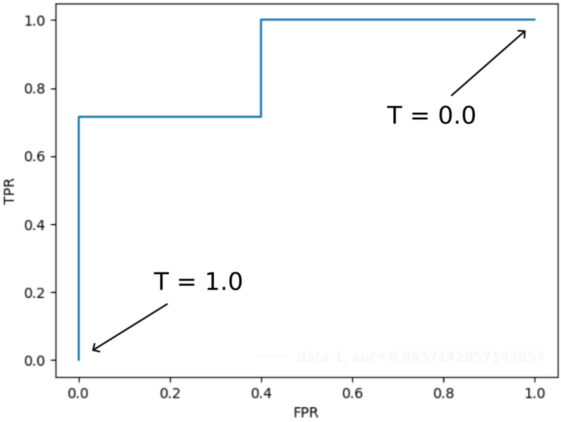
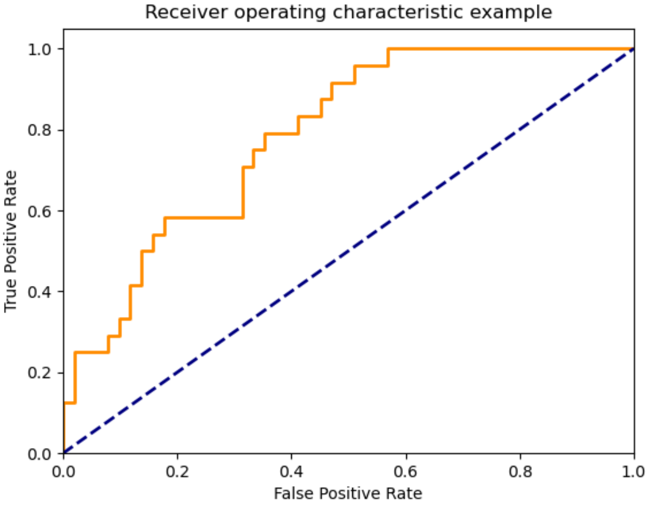


ROC-AUC $= 0.8857$

Iris - ROC-AUC



ROC-AUC $= 0.79$

ROC-AUC - Probabilistic Interpretation

How is the ROC-AUC connected with the samples?

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Consider our cancer detection example:

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The ROC-AUC is the probability of succeeding in the $h_i \geq h_j$ test.

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  Accuracy, Precision, Recall, F_1, and few more
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- probabilistic classifiers,
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There are still several questions unanswered:

- When to use the metrics.
- How to estimate the influence of sampling the dataset.

Use of Evaluation Metrics

In our case, the following scenarios are typical:

- **Final test**: Evaluate the model on the test set (separated at the beginning of training) and then compute the metrics. May inform the user about the quality of the model.

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  There are (at least) two scenarios in which this happens:
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  - Hyperparameter fine-tuning.
  - Comparison of different models (e.g., KNN and decision trees).

Keep in mind that the metrics are artificial, and the results of the model are roughly summarized.

It would be best if you always strived to test the proper functionality of your model in as natural conditions as possible.

For example, a model for medical diagnosis should be evaluated by medical doctors who may observe many features of its behavior that are difficult to express quantitatively.

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We will consider these issues in some later lecture. Concretely,

- *Bias-variance* tradeoff
- *Statistical tests* for testing
  - significance of the metrics values,
  - paired t-tests for comparing models.

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How to compare $(\mathrm{Precision}_1, \mathrm{Recall}_1)$ of the fist classifier with $(\mathrm{Precision}_2, \mathrm{Recall}_2)$ of the second classifier?

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Let us consider two classifiers. How do you compare them?

Accuracies and F_1 scores can be compared easily (they are just numbers).

How to compare $(\text{Precision}_1, \text{Recall}_1)$ of the fist classifier with $(\text{Precision}_2, \text{Recall}_2)$ of the second classifier?

Thresholding

- Introduce a threshold $0 \leq t \leq 1$
- Demand, one of the two metrics (typically the Recall), to be at least t. That is

$$\text{Recall}_1 \geq t \qquad \text{Recall}_2 \geq t$$

- Compare the values of the other metric numerically. In our case, decide whether

$$\text{Precision}_1 \geq \text{Precision}_2$$

(Still need to be concerned about the statistical significance.)

Example

Actual condition	**Predicted condition**	
	Canc.	**Non-canc.**
Cancer	6	2
Non-canc.	1	3
Total	$8 + 4 = 12$	

Actual condition	**Predicted condition**	
	Canc.	**Non-canc.**
Cancer	5	3
Non-canc.	0	4
Total	$8 + 4 = 12$	

$$\text{Precision}_1 = \frac{6}{7} \qquad \text{Recall}_1 = \frac{6}{8}$$

$$\text{Precision}_2 = \frac{5}{5} = 1 \qquad \text{Recall}_2 = \frac{5}{8}$$

Consider a threshold t on the Recall.

The second classifier is better if the threshold t is $5/8$, then the second classifier is better.

If the threshold t is $6/8$, then the second classifier is unacceptable.