Applied Machine Learning - Basic

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Lecture 6

Data Science and Computation PhD + Master in Bioinformatics

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Communications

2 bonus virtual lectures! incl. notebooks!

Focus on:

- **Matplotlib**
  - https://unibo.cloud.panopto.eu/Panopto/Pages/Viewer.aspx?id=65556357-e7c9-42aa-aa31-ae6c0162120a#
- **Seaborn**
  - https://unibo.cloud.panopto.eu/Panopto/Pages/Viewer.aspx?id=f4198b86-9440-4568-8583-ae6c01529aec#

Recap

(…)

Advices for applying ML

- Evaluating a learning model → Evaluate an hypothesis
- Model selection and TVT sets
- Bias vs variance diagnosis
- Regularisation and bias vs variance
- Learning curves

NEXT:

Performance metrics and skewed classes

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We've talked about **how to evaluate learning algos**, talked about **model selection**, talked a lot about **bias and variance**.

So how does this help us figure out what are potentially fruitful things to try to do to improve the performance of a learning algorithm?

Let's go back to our original motivating example and then go straight to the result.

Debugging a learning algo

Suppose you have implemented regularised linear regression to predict housing prices. However, when you test your hypothesis on a new set of houses, you find that it makes unacceptably large errors in its predictions. What should you try next?

We discussed:

- getting more training examples
- try smaller sets of features
- try getting additional features
- try adding polynomial features (squares, cross products, etc)
- try increasing/decreasing lambda

Let's revisit them in view of what we now know a bit more.

What to try next

- getting more training examples —> **CHECK YOUR VARIANCE**
  - good to fix high-variance problems (i.e. your CV error is quite bigger than training error)
  - but if you have high bias, this will not help, so do <u>not</u> waste time in collecting more examples..
- try smaller sets of features
  - good to fix high-variance problems
  - but if you have high bias, this will not help, so do <u>not</u> waste time in carefully selecting features…
- try getting additional features
  - good to fix high-bias problems (h too simple, so add features to make h more able to fit the training set)
- try adding polynomial features (squares, cross products, etc)
  - another way to fix high-bias problems
- try increasing lambda
  - good to fix high-variance problems
- try decreasing lambda
  - good to fix high-bias problems

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No deep preliminary discussion on error analysis and the importance of having error metrics, but <u>use of intuition</u> that it is of **great importance to have a single real number evaluation metric for a learning algorithm**.

In most cases, **accuracy** is just fine. But there is one and common important case, where it is particularly tricky to come up with an appropriate evaluation metric. That is the case of so-called **skewed classes**.

Consider the problem of cancer classification, where we have features of medical patients and we want to decide whether or not they have cancer.

Example : cancer/not-cancer classification

→ train a logistic regression model $h_\theta(x)$ ⇒ a classifier

$$y = \{0, 1\}$$

benign malignant

→ test your classifier : e.g. find a 1% error on test set

⇒ impressive ! 99% correct diagnosis !

Example : malignant / benign classification

→ train a logistic regression model $h_\theta(x)$ ⇒ a classifier

$y = \{0, 1\}$

benign malignant

→ test your classifier : e.g. find a 1% error on test set

⇒ impressive ! 99% correct diagnosis !

→ suppose you find out that only 0.5% of patients have cancer
(eg you assign $y=0$ to everyone and you are wrong in 0.5% of the cases)

⇒ no longer impressive :(

if you IGNORE features x, you do even better !
("non learning algo")

When a non-learning algo does a good job, better than a simple learning algo, we are in peculiar case:

always "y=0" or
always "y=1"

positive examples
<<
negative examples

=> "skewed classes"

When a non-learning algo does a good job, better than a simple learning algo, we are in peculiar case:

always "y=0" or
always "y=1"

positive examples << negative examples ⇒ "skewed classes"

This poses a tricky question:

if I go from a learning algo at 99.1% accuracy (0.9% error) to one at 99.7% accuracy (0.3% error), how can I be sure the latter is an improvement, or a random mod that e.g. predicts =0 more often and I am in skewed classes scenario?

With skewed classes, accuracy ↗ is not always an indicator of improvements in the classifier

You need a different error metric → PRECISION / RECALL

Precision / Recall

actual → / predicted ↓	1	0
1		
0		

Precision / Recall

predicted ↓ \ actual →	1	0
1	TRUE POSITIVE	
0		TRUE NEGATIVE

Precision / Recall

predicted ↓ \ actual →	1	0
1	TRUE POSITIVE	FALSE POSITIVE
0	FALSE NEGATIVE	TRUE NEGATIVE

Precision / Recall

predicted ↓ \ actual →	1	0
1	TRUE POSITIVE	FALSE POSITIVE
0	FALSE NEGATIVE	TRUE NEGATIVE

NOTE :

- TRUE vs FALSE
  → position in the matrix
  ⇒ depends on "predicted" and "actual"

- POSITIVE vs NEGATIVE
  → depends on "predicted" only

Precision / Recall

predicted ↓ \ actual →	1	0
1	TP	FP
0	FN	TN

PRECISION

"Among all patients predicted to have cancer, how many actually have it?"

→ how "precise" have you been?

$$\Rightarrow \frac{\#\ TP}{\underbrace{\#\ \text{predicted } P}_{TP+FP}} = \frac{TP}{TP+FP}$$

better if this is high!

Precision / Recall

predicted ↓ \ actual →	1	0
1	TP	FP
0	FN	TN

PRECISION

"Among all patients predicted to have cancer, how many actually have it?"

$$\stackrel{\text{def}}{=} \frac{TP}{\underbrace{TP+FP}_{\text{predicted P}}} \quad \text{(should be as high as possible!)}$$

RECALL

"Among all patients that actually have cancer, how many did we predict to have it?"

→ "how many of the TP were "recalled" (found)?"

$$\Rightarrow \frac{\cancel{\#}\ TP}{\cancel{\#}\ \text{actual } P} = \frac{TP}{TP+FN}$$

better if this is high!

Precision / Recall

predicted ↓ \ actual →	1	0
1	TP	FP
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PRECISION

"Among all patients predicted to have cancer, how many actually have it?"

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RECALL

"Among all patients that actually have cancer, how many did we predict to have it?"

$$\stackrel{\text{def}}{=} \frac{TP}{\underbrace{TP+FN}_{\text{actual P}}} \quad \text{(should be as high as possible!)}$$

Precision / Recall

$$\text{PRECISION} \stackrel{\text{def}}{=} \frac{TP}{TP+FP}$$

Intuitively: the **precision** is the ability of the classifier not to label as positive a sample that is negative.

$$\text{RECALL} \stackrel{\text{def}}{=} \frac{TP}{TP+FN}$$

Intuitively: the **recall** is the ability of the classifier to find all the positive samples.

predicted \ actual	1	0
1	TP	FP
0	FN	TN

Example :

classifier that predicts $y=0$ always :

$\Rightarrow$ $TP = 0$ $\Rightarrow$ PRECISION $= 0$

RECALL $= 0$

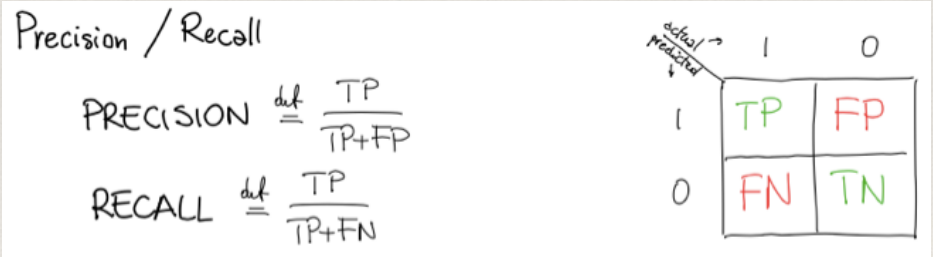
C.Y.U.

Quiz

Your algorithm has a performance on the test set given by this matrix.
What is the algo's **precision**?

	1	0
1	80	20
0	80	100

- 0.5
- 0.8
- 0.08
- 0.1



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Precision / Recall

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Precision / Recall

$$\text{PRECISION} \stackrel{def}{=} \frac{TP}{TP+FP}$$

$$\text{RECALL} \stackrel{def}{=} \frac{TP}{TP+FN}$$

actual → / predicted ↓	1	0
1	TP	FP
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C.Y.U.

Quiz

Same as before. What is the algo's **recall**?

- **0.5**
- 0.8
- 0.08
- 0.1

	1	0
1	80	20
0	80	100

Precision / Recall

$$\text{PRECISION} \stackrel{def}{=} \frac{TP}{TP+FP}$$

$$\text{RECALL} \stackrel{def}{=} \frac{TP}{TP+FN}$$

predicted ↓ / actual →	1	0
1	TP	FP
0	FN	TN

When we define **precision** and **recall**, usually we use the convention that y is equal to 1 in the presence of the *more rare class*.

- So if we are trying to detect rare conditions such as cancer, hopefully that's a rare condition, precision and recall are defined setting y = 1, rather than y = 0: the presence of the rare class is the driver.

Summary

As we were not satisfied about “accuracy” only, as it could be cheated easily by a non-learning algo, we introduced **precision** and **recall**.

Now, more generally, even for settings where we have very skewed classes, it is not possible for an algorithm to"cheat" and somehow get a very high precision and a very high recall by doing some simple thing like predicting y=0 (or y=1) all the time.

We now are more confident to state if a classifier is actually a good classifier: **precision/recall are more useful evaluation metrics to tell if one algorithm may be doing well in real applications**.

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We talked about precision and recall as evaluation metrics for classification problems with skewed constants.

For many applications, we'll want to somehow control the **trade-off between precision and recall**.

Cancer example $\rightarrow$ train logistic regression

$$\text{PRECISION} \stackrel{\text{def}}{=} \frac{TP}{\underbrace{TP+FP}_{\text{predicted P}}}$$

$$\text{RECALL} \stackrel{\text{def}}{=} \frac{TP}{\underbrace{TP+FN}_{\text{actual P}}}$$

$$0 \leq h_\theta(x) \leq 1$$

$$\text{predict} \begin{cases} 1 & \text{if } h_\theta(x) \geq 0.5 \\ 0 & \text{if } h_\theta(x) < 0.5 \end{cases}$$

this classifier will give me some values for

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Suppose we want to predict $y=1$ only if we are VERY confident

e.g.

$$\begin{cases} 1 & \text{if } h_\theta(x) \geq \cancel{0.5} \quad 0.7 \\ 0 & \text{if } h_\theta(x) < \cancel{0.5} \quad 0.7 \end{cases}$$

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more "precise"!

$\Rightarrow$ higher precision

I do not know TP (numerator), but for sure predicted P ($=TP+FP$) ↘

$\Rightarrow$ denominator ↘ $\Rightarrow$ **precision** ↗

Cancer example → train logistic regression

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more "precise"!

I "recall" (find) less TP w.r.t. before

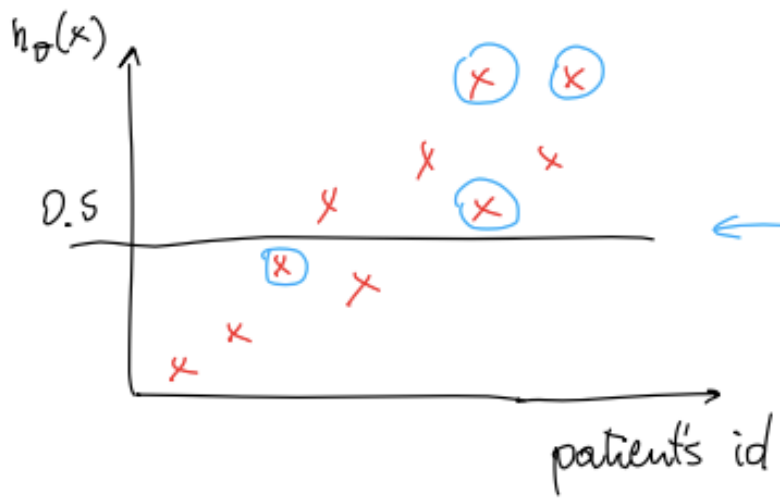
$\Rightarrow$ higher precision, but lower recall

I do not know TP (numerator), but for sure predicted P ($=TP+FP$) ↘
$\Rightarrow$ denominator ↘ $\Rightarrow$ **precision** ↗

Now predicting $y=1$ on a smaller # patients
I increased the purity of the sample:
TP (numerator) ↘, plus FN at the denominator ↗ $\Rightarrow$ **recall** ↘

Let's check with an example

Example :



× value of $h_\theta(x)$ for a patient

⊗ same, but this has cancer

threshold at 0.5

actual / predicted	1	0
1	TP	FP
0	FN	TN

Example :

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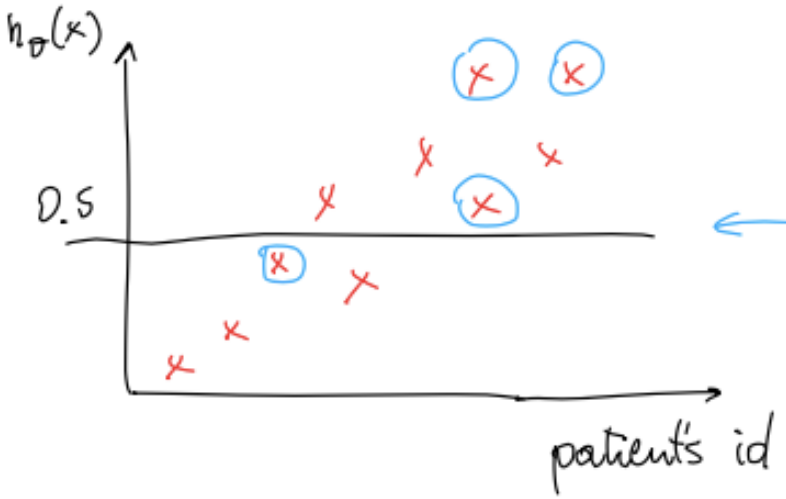


threshold at 0.5

actual → / predicted ↓	1	0
1	TP	FP
0	FN	TN

$$\text{PRECISION} \triangleq \frac{TP}{\underbrace{TP+FP}_{\text{predicted P}}}$$

$$\text{RECALL} \triangleq \frac{TP}{\underbrace{TP+FN}_{\text{actual P}}}$$

0.5 ⇒

actual → / predicted ↓	1	0
1	3	3
0	1	3

⇒

$$\text{Precision} = \frac{3}{3+3} = 0.5$$

only 50% of selected have cancer

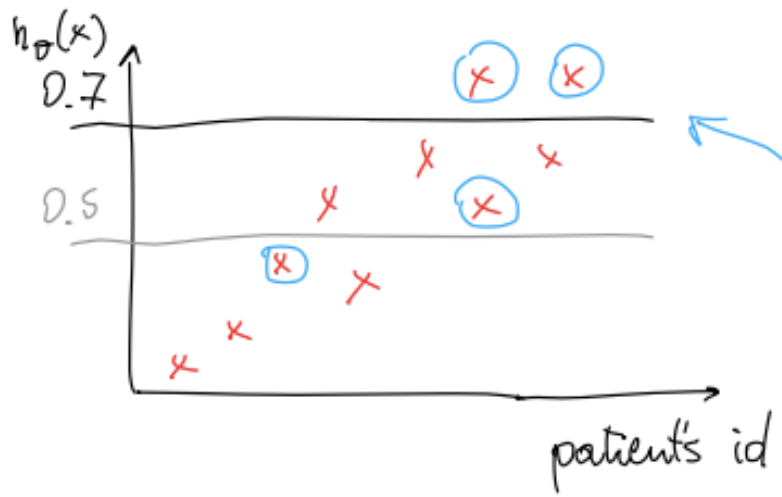
$$\text{Recall} = \frac{3}{3+1} = 0.75$$

I selected 3/4 of them

Example :

× value of $h_\theta(x)$ for a patient

⊗ same, but this has cancer



threshold at 0.7

actual → / predicted ↓	1	0
1	TP	FP
0	FN	TN

$$\text{PRECISION} \triangleq \frac{TP}{\underbrace{TP+FP}_{\text{predicted P}}}$$

$$\text{RECALL} \triangleq \frac{TP}{\underbrace{TP+FN}_{\text{actual P}}}$$

0.7 ⇒

actual → / predicted ↓	1	0
1	2	0
0	2	6

⇒

$$\text{Precision} = \frac{2}{2+0} = 1$$ perfect!

$$\text{Recall} = \frac{2}{2+2} = 0.5$$ I selected 50% of them

Example summary :

	prec	recall
0.5 →	0.5	0.75
0.7 →	1.0	0.5

⇓ prec ↗

⇓ recall ↘

Cancer example → Train logistic regression

$$\text{PRECISION} \stackrel{\text{def}}{=} \frac{TP}{\underbrace{TP+FP}_{\text{predicted P}}}$$

$$\text{RECALL} \stackrel{\text{def}}{=} \frac{TP}{\underbrace{TP+FN}_{\text{actual P}}}$$

$$0 \leq h_\theta(x) \leq 1$$

$$\text{predict} \begin{cases} 1 & \text{if } h_\theta(x) \geq \cancel{0.5} \quad \cancel{0.7} \quad 0.9 \\ 0 & \text{if } h_\theta(x) < \cancel{0.5} \quad \cancel{0.7} \quad 0.9 \end{cases}$$

We can push this further ↗ ⇒ predict $y=1$ ONLY IF we are 90% certain it is cancer

⇐ a large fraction of those patients will turn out to have cancer

(again) ⇒ even higher precision and even lower recall

Suppose instead you have a different goal: you want to avoid missing too many cases of cancer $\longrightarrow$ i.e. avoid FN

[NOTE: as a real-life example, it is compelling to fight FN, i.e. sick but no diagnosis!
In other words, when in doubt, trigger $y=1$ so they make exams and figure out...]

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In this case, you need a lower threshold instead:

$$0 \leq h_\theta(x) \leq 1$$

$$\text{predict} \begin{cases} 1 & \text{if } h_\theta(x) \geq \cancel{0.5} \;\; 0.3 \\ 0 & \text{if } h_\theta(x) < \cancel{0.5} \;\; 0.3 \end{cases}$$

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$\Rightarrow$ lower precision and higher recall

a larger fraction of patient we are saying to have cancer will eventually turn out not to have it

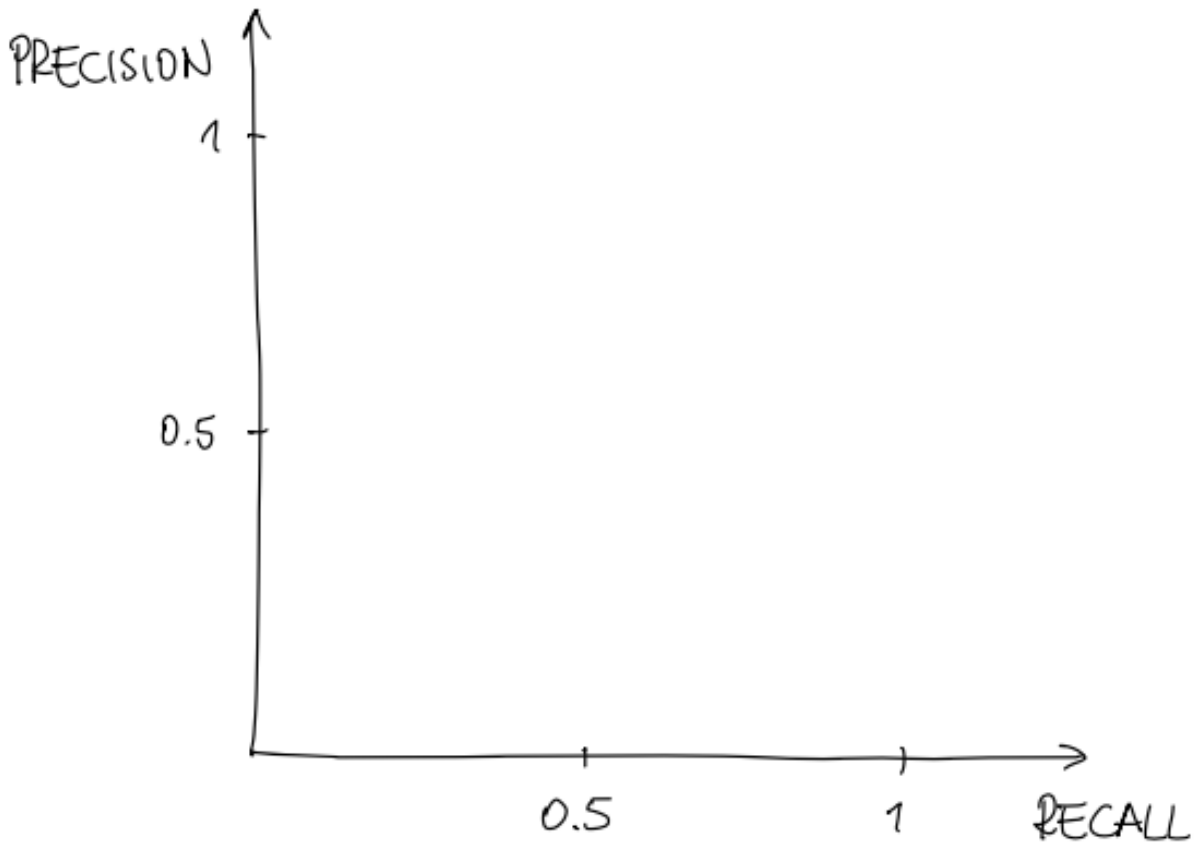
we are going to correctly flagging a larger fraction of patients that actually do have cancer

If this threshold can be different from 0.5 - and there seems to be a motivation - is there a way to choose this threshold automatically?

Or - more generally - if we leave this open, how do we compare different models having different precision/recall values?

More generally : predict $y=1$ if $h_\theta(x) \geq$ "threshold"

For most classifiers there is a <u>trade-off</u> between precision and recall, and as you vary the threshold you can plot some curve



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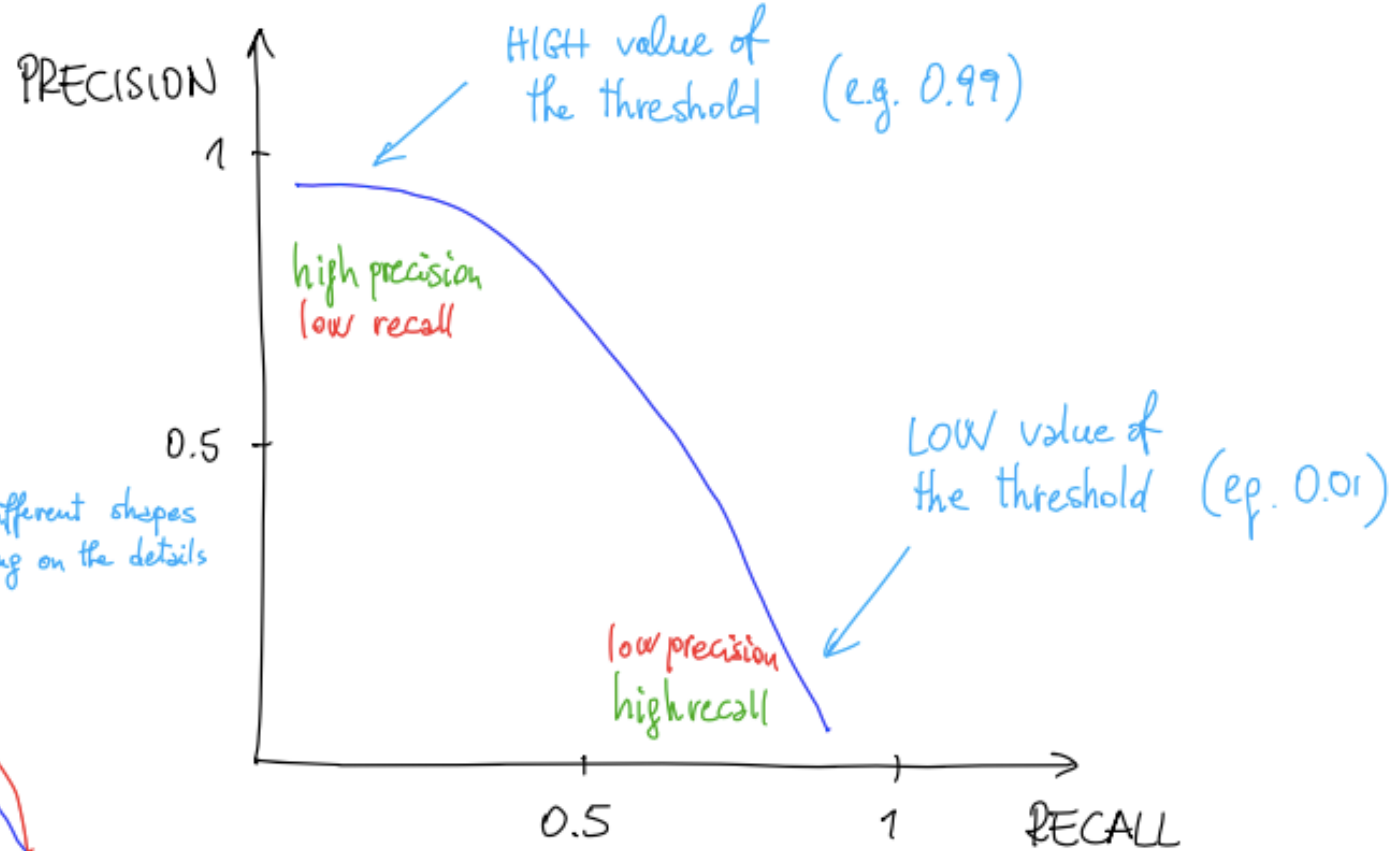
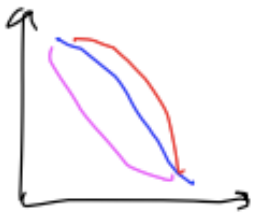


NOTE : many different shapes possible, depending on the details of the classifiers.



Suppose you have either a) 3 different algos
b) same algo but with 3 different thresholds

	PRECISION (P)	RECALL (R)
algo 1	0.5	0.4
algo 2	0.7	0.1
algo 3	0.02	1.0

would it be easier to just have 1 number, then? (i.e. accuracy)

How do you decide which is best ?
(BTW, we now have 2 raw nbs and not just 1 as metric...)

You can try : average $= \frac{P+R}{2}$

Suppose you have either a) 3 different algos
b) same algo but with 3 different thresholds

	PRECISION (P)	RECALL (R)	average
algo 1	0.5	0.4	0.45
algo 2	0.7	0.1	0.4
algo 3	0.02	1.0	0.51

How do you decide which is best?

You can try : average = $\cancel{\frac{P+R}{2}}$

→ not so good. Best is algo 3, an extreme, that predicts $y=1$ all the time... Not a great way to select the best classifier.

Suppose you have either a) 3 different algos
b) same algo but with 3 different thresholds

	PRECISION (P)	RECALL (R)	F1 score	
algo 1	0.5	0.4	0.444	best
algo 2	0.7	0.1	0.175	
algo 3	0.02	1.0	0.0392	worst

Introduce F1 score (F score), a way to combine P and R:

$$F_1 \text{ score} \overset{\text{def}}{=} 2\,\frac{P \cdot R}{P+R}$$

(just one way!)
→ hystorical...

if one is 0 ⇒ $F_1 = 0$ (~same if small)
Both need to be largish for a good F1

$P=0$ or $R=0 \Rightarrow F_1 = 0$
$P=1$ and $R=1 \Rightarrow F_1 = 1$

Suppose you have either a) 3 different algos
b) same algo but with 3 different thresholds

	PRECISION (P)	RECALL (R)	F1 score	
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Introduce F1 score (F score), a way to combine P and R:

$$F_1 \text{ score} \overset{\text{def}}{=} 2\,\frac{P \cdot R}{P+R}$$

Intuitively: the **F1** can be interpreted as a weighted harmonic mean of precision and recall (best at 1 and worst at 0)

(just one way!) → historical...

if one is 0 ⇒ $F_1 = 0$ (~same if small)
Both need to be largish for a good F1

$P=0$ or $R=0$ ⇒ $F_1 = 0$
$P=1$ and $R=1$ ⇒ $F_1 = 1$

Summary

We discussed the notion of trading off between **precision** and **recall**, and how we can vary the threshold that we use to decide whether to predict y=1 or y=0. By varying the threshold, you can control such trade off

- e.g. "we need to be at least 70% confident or 90% confident in order to predict y=1"

We discussed about the **F1** scorer, a single real number evaluation metric whose definition is based on precision and recall.

If your goal is to automatically set that threshold to decide what's really y=1 vs y=0, one reasonable way to do so would be:

- to try a range of different values of thresholds
- to evaluate these different thresholds on your cv set
- to pick whatever value of threshold gives you the highest F1 score

This is a reasonable way to automatically choose the threshold for your classifier.

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Re-visit with your memory the “metrics” discussion we had

- accuracy enough or not, more metrics, which ones, etc..

We add few details, in a few simple slides.

ROC curve

Are you comfortable with performance parameters whose values change according to the classification threshold?

A **ROC curve** (**Receiver Operating Characteristic curve**) is a graph showing the performance of a classification model <u>at all classification thresholds</u>.

It is a curve in the TPR-FPR space:

$$\text{True Positive Rate } (\mathbf{TPR}) = \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{False Positive Rate } (\mathbf{FPR}) = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

Reminder:

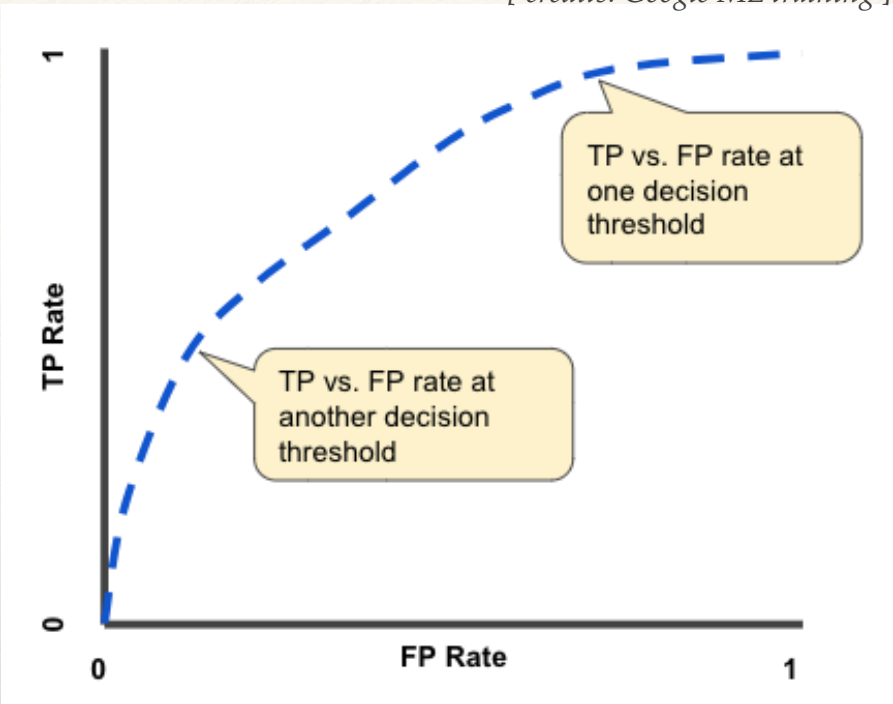
$$\text{PRECISION} \stackrel{\text{def}}{=} \frac{\text{TP}}{\underbrace{\text{TP}+\text{FP}}_{\text{predicted P}}}$$

$$\text{RECALL} \stackrel{\text{def}}{=} \frac{\text{TP}}{\underbrace{\text{TP}+\text{FN}}_{\text{actual P}}}$$

An ROC curve plots TPR vs. FPR at different classification thresholds.

- every point on the ROC curve corresponds to just one value of the classification threshold
- e.g. lowering the classification threshold classifies more items as positive, thus increasing both False Positives and True Positives.

[credits: Google ML training]



To compute the points in an ROC curve, we could evaluate a logistic regression model many times with different classification thresholds

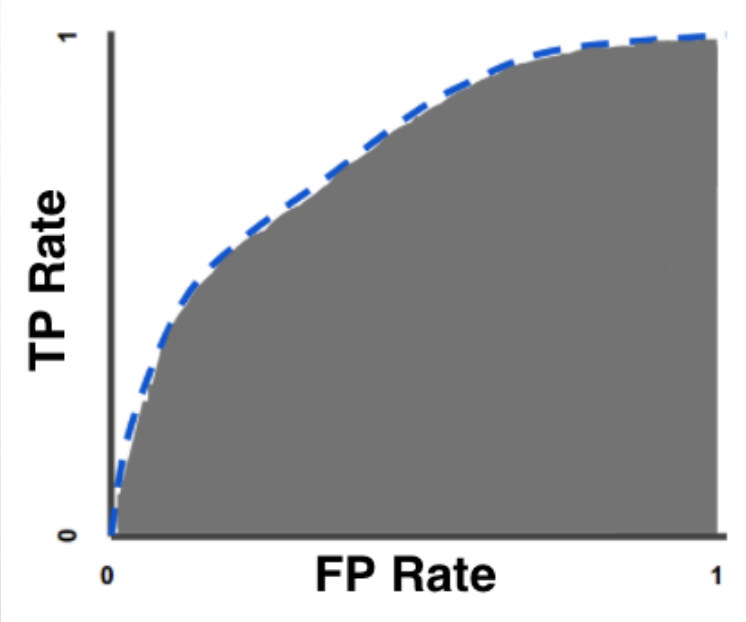
- but this would be inefficient..

Fortunately, there's an efficient, sorting-based algorithm that can provide this information for us, called **AUC**.

AUC: Area Under the ROC Curve

AUC ("**Area under the ROC Curve**") measures the entire two-dimensional area underneath the entire ROC curve from (0,0) to (1,1)

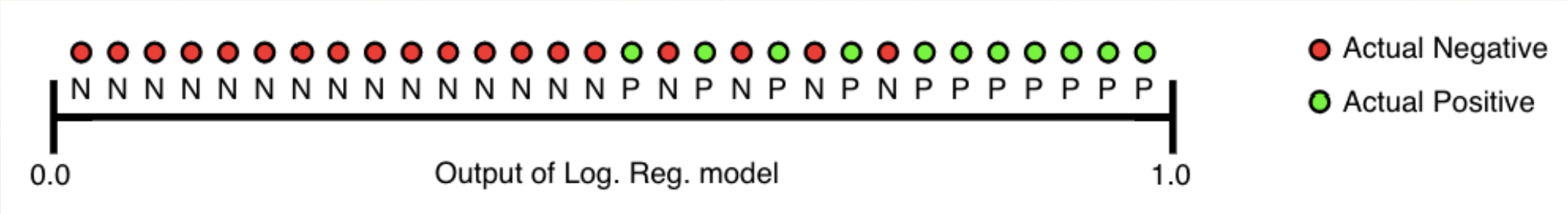
AUC provides an aggregate measure of performance across all possible classification thresholds.



AUC ranges in value from 0 to 1

- a model whose predictions are **100% correct** has **AUC = 1.0**
- a model whose predictions are **100% wrong** has **AUC = 0.0**

AUC: Area Under the ROC Curve



One way of interpreting AUC is as *the probability that the model ranks a random positive example "higher" than a random negative example*

- E.g. take the example above, which are arranged from left to right in ascending order of logistic regression predictions: AUC represents the probability that a random positive (green) example is positioned to the right of a random negative (red) example example

Why AUC?

AUC is desirable for the following two reasons:

- AUC is **classification-threshold-invariant**. It measures the quality of the model's predictions irrespective of what classification threshold is chosen.
- AUC is **scale-invariant**. It measures how well predictions are ranked, rather than their absolute values.

However, both these reasons come with caveats, which may limit the usefulness of AUC in certain use cases:

- **Classification-threshold invariance is not always desirable**. In cases where there are wide disparities in the cost of false negatives vs. false positives, it may be critical to minimise one type of classification error
  - e.g. when doing email spam detection, you likely want to prioritise minimising FP (even if that results in a significant increase of FN). AUC isn't a useful metric for this type of optimisation.
- **Scale invariance is not always desirable**. For example, sometimes we really do need well-calibrated probability outputs, and AUC won't tell us about that.

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Hands-on:

3 - Data prep - explore data (part 2)

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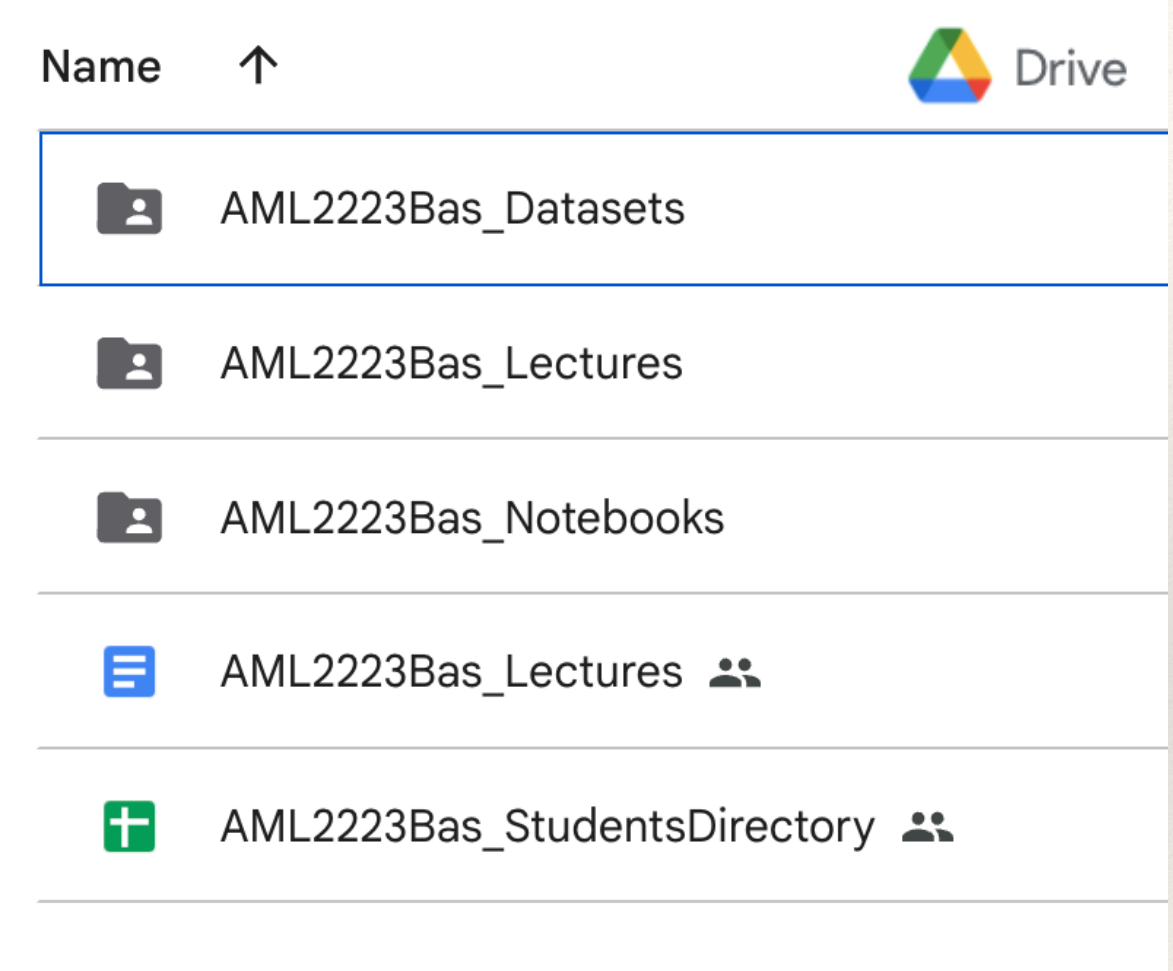
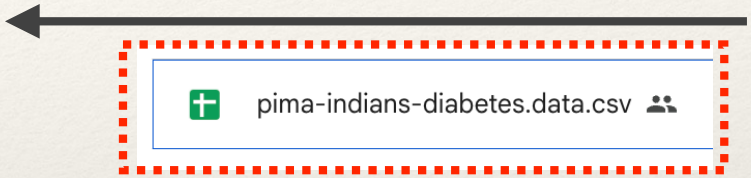
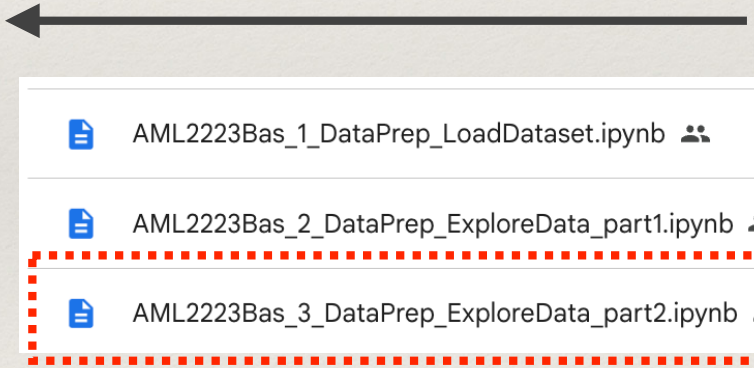
Look into these:







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Hands-on:

4 - Data prep - Prepare data

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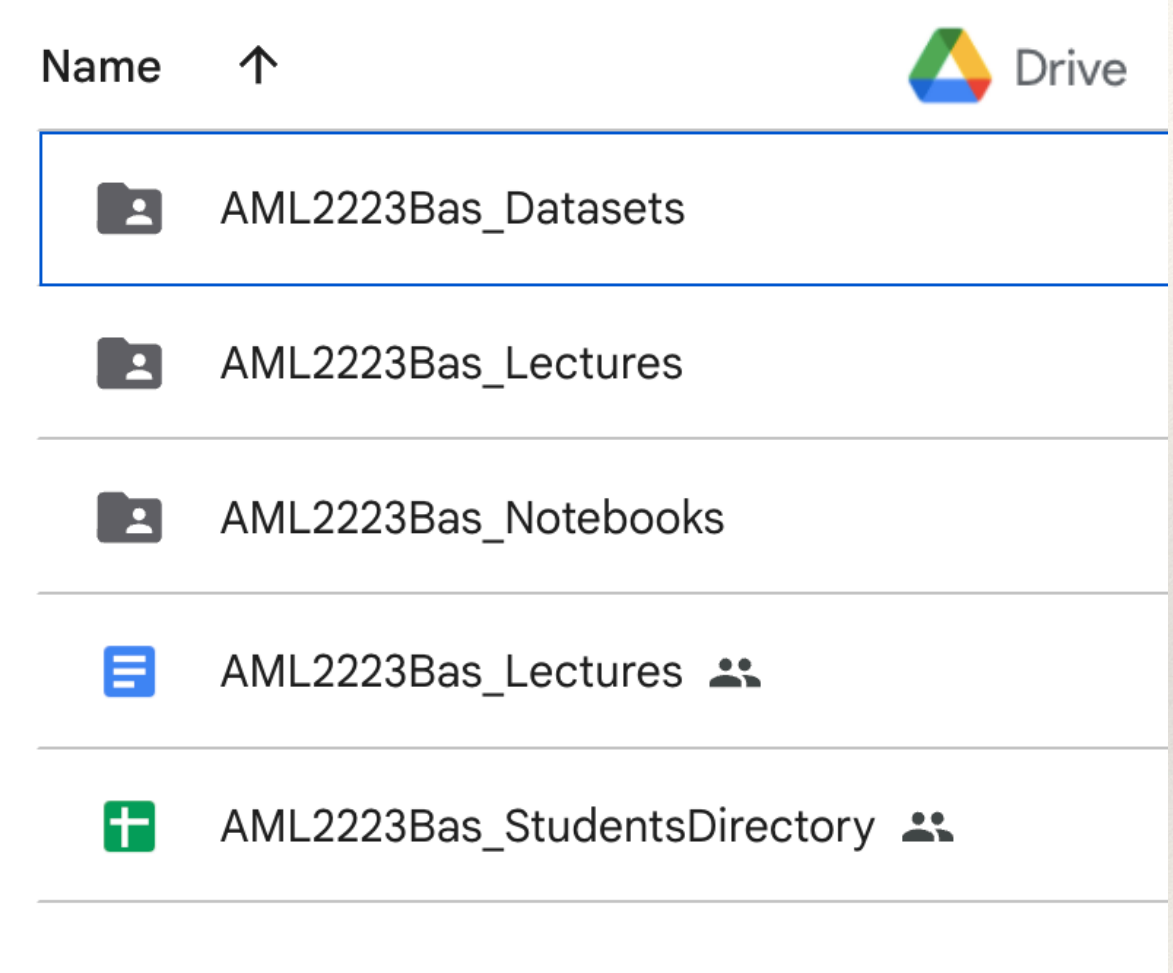

Notebook nb.4

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Hands-on:

5 - Data prep - Feature selection

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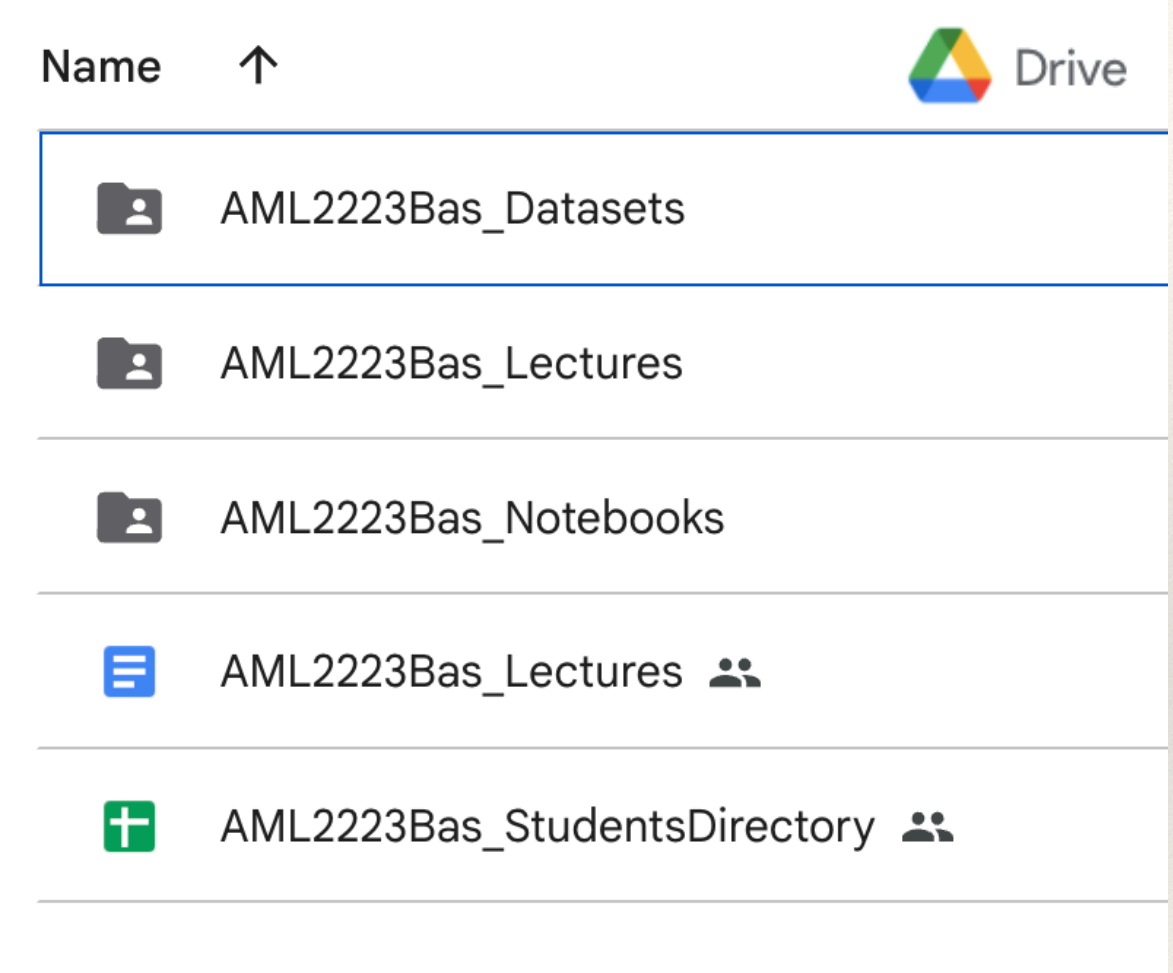

Notebook nb.5