Beginner-friendly ML school: Performance Metrics

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Beyond accuracy

Imagine building an algorithm to look for rare objects (e.g. habitable planets).
The data contains 1,000 instances.
Of those, 10 belong to the “interesting” class.
(the data set is imbalanced: the target values are not distributed uniformly).
You feel lazy and submit an algorithm that says that there are no habitable planets.

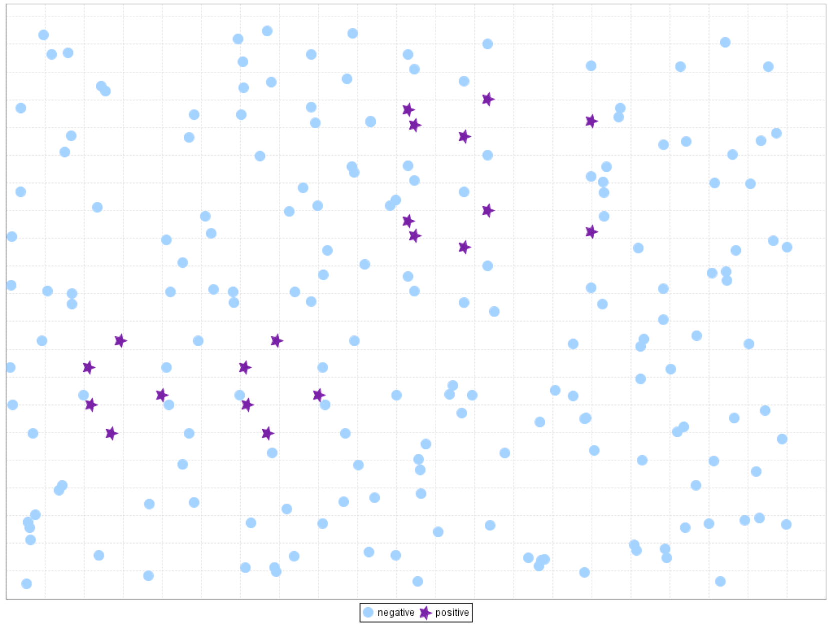
What is its accuracy (% of correct predictions)?

Picking a performance metric

"The accuracy paradox"

Accuracy = % of correct predictions

meaningless in unbalanced data set

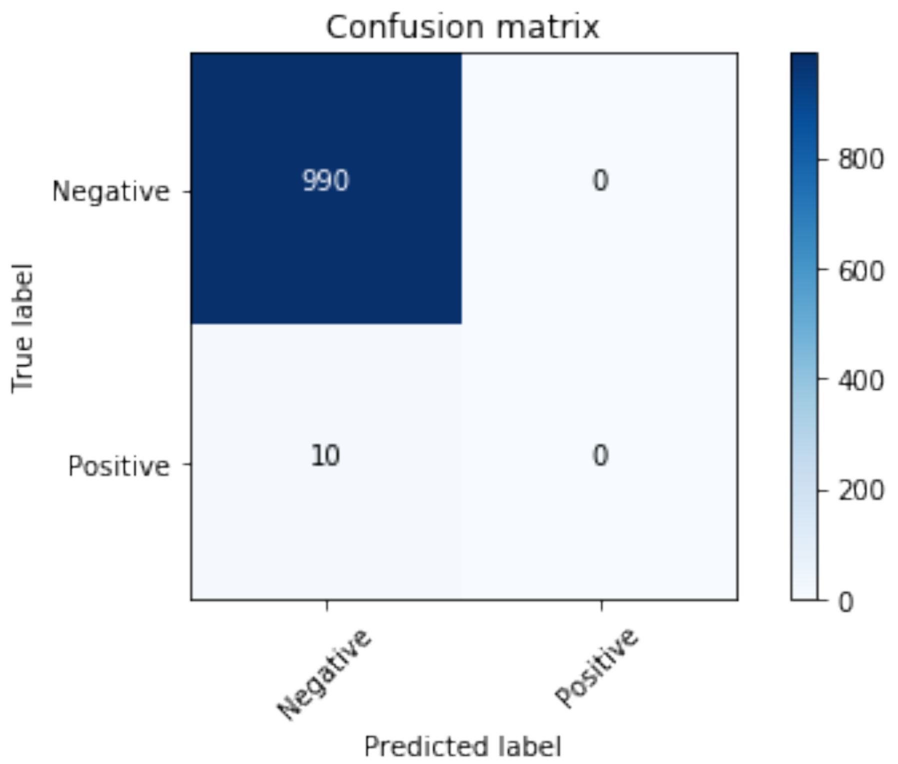


For our dataset :
Accuracy = 990/1000 = 99.0%!

Evaluating classifiers performance: beyond accuracy

For a binary classifier where the "true" or desired class members are defined to be positive, every metric is enclosed by four numbers:

TP = True Positives	0
TN = True Negatives	990
FP = False Positives	0
FN = False Negatives	10



Accuracy = % of correct predictions **TP+TN/(TP+TN+FP+FN)**

Alternative metrics

precision = percentage of correct positive classifications TP/(TP + FP)

recall = percentage of “caught” positive instances = TP/(TP+FN)

For our lazy classifier

TP = 0; TN = 990; FP = 0; FN = 10

Will have undefined precision and 0 recall
so we’ll be able to know that something is amiss.

Alternative metrics

Often we (astronomers) talk of precision as purity, or 1 – precision as contamination

Recall is IMO best visualized as completeness

Another common one is F1 = weighted avg of precision/recall

The best metric can only be decided by you on the basis of the science you want to do!

A few words about ROC and AUC

**ROC (receiving operator characteristic) is
a plot of TPR (True Positive Rate) vs FPR (False Positive Rate)**

TPR = TP/(TP+FN) = recall

**FPR = FP/(TN+FP)
(swap F->T in recall)**

How can this be a plot?

**The trick is to calculate it for different thresholds
of what it means for an object to belong to the positive class
(as opposed to the "standard" 0.5)**

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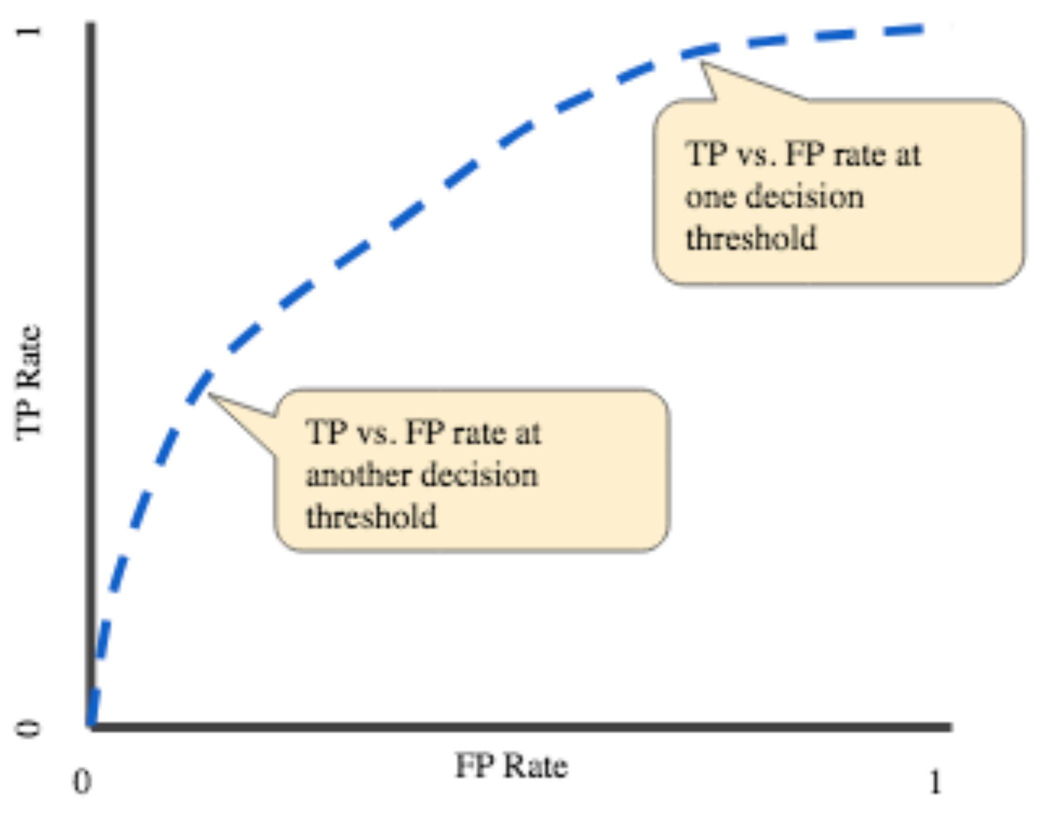
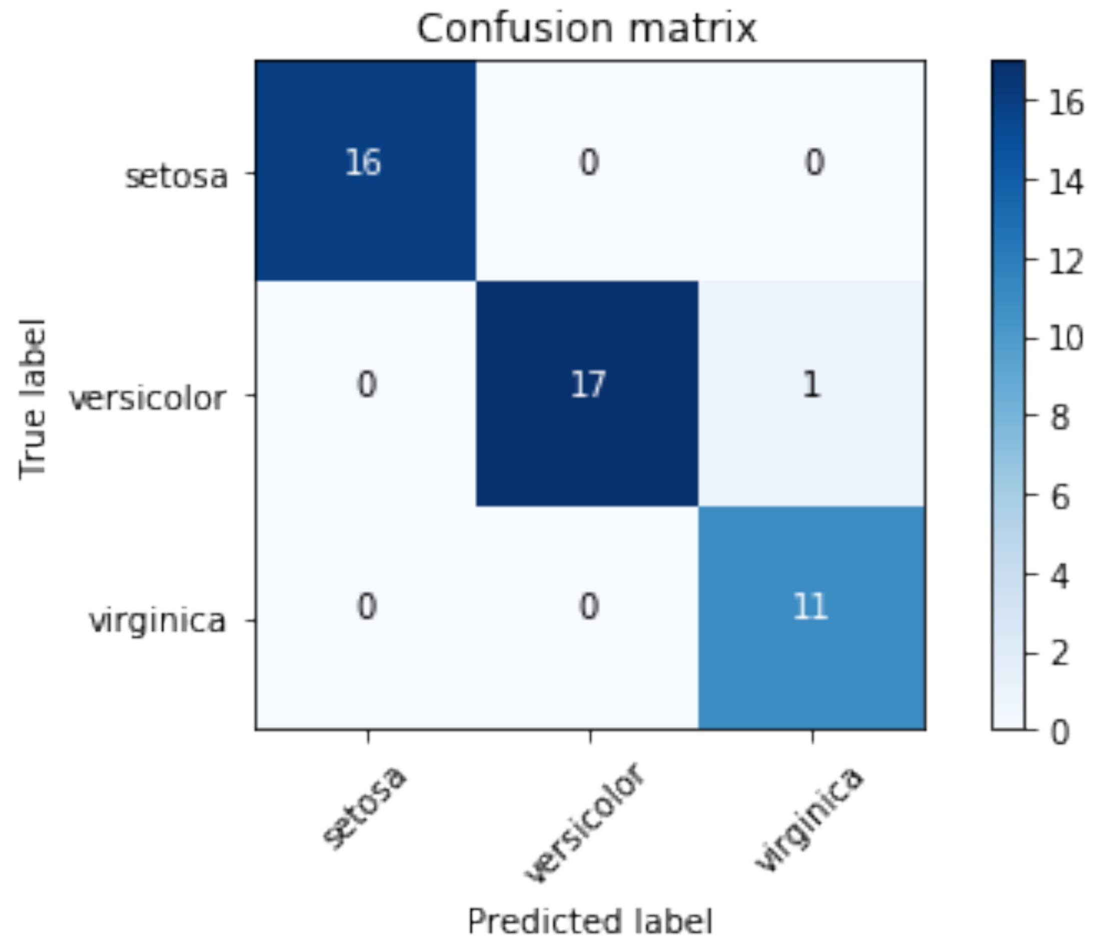


AUC = area under the curve

What happens for non-binary classifiers?

The confusion matrix can be built normally

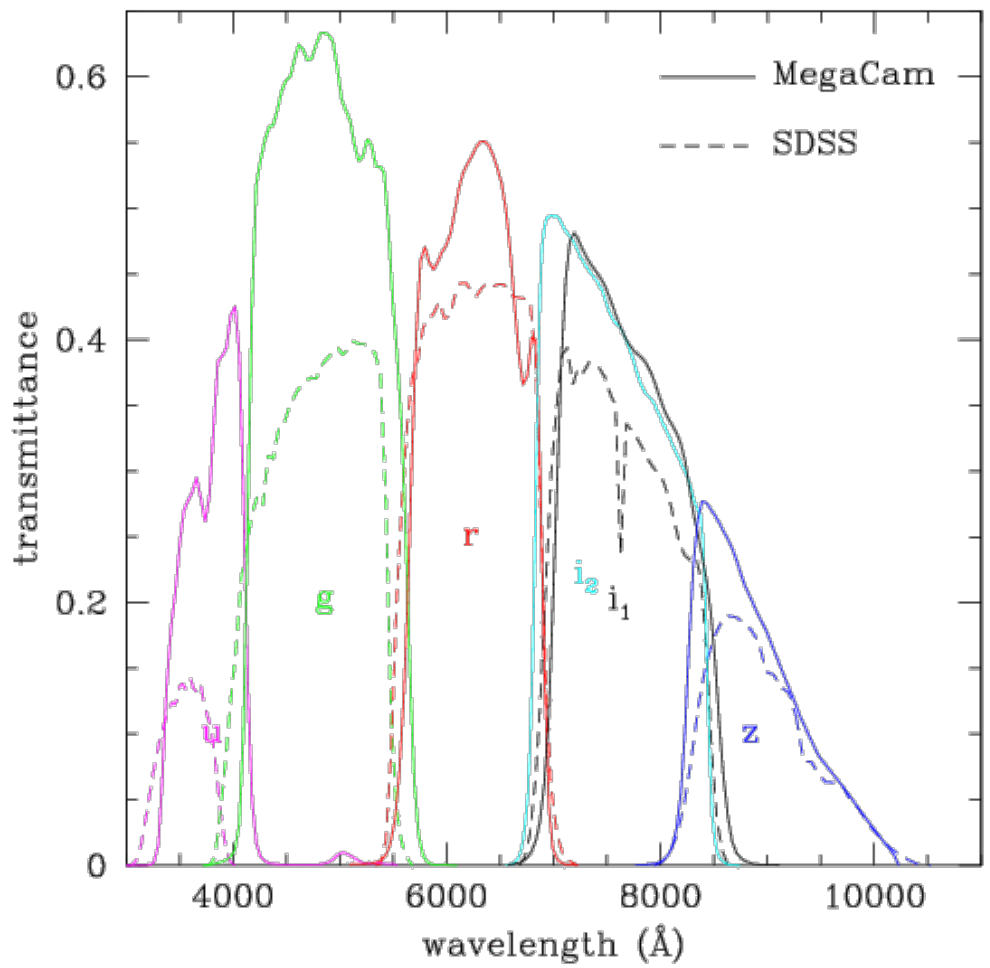


Note: in this case accuracy is still the % of correct predictions, but precision and recall require you to define a "positive" class and do one-vs-all (plus choose micro/macro averaging if you want one number)

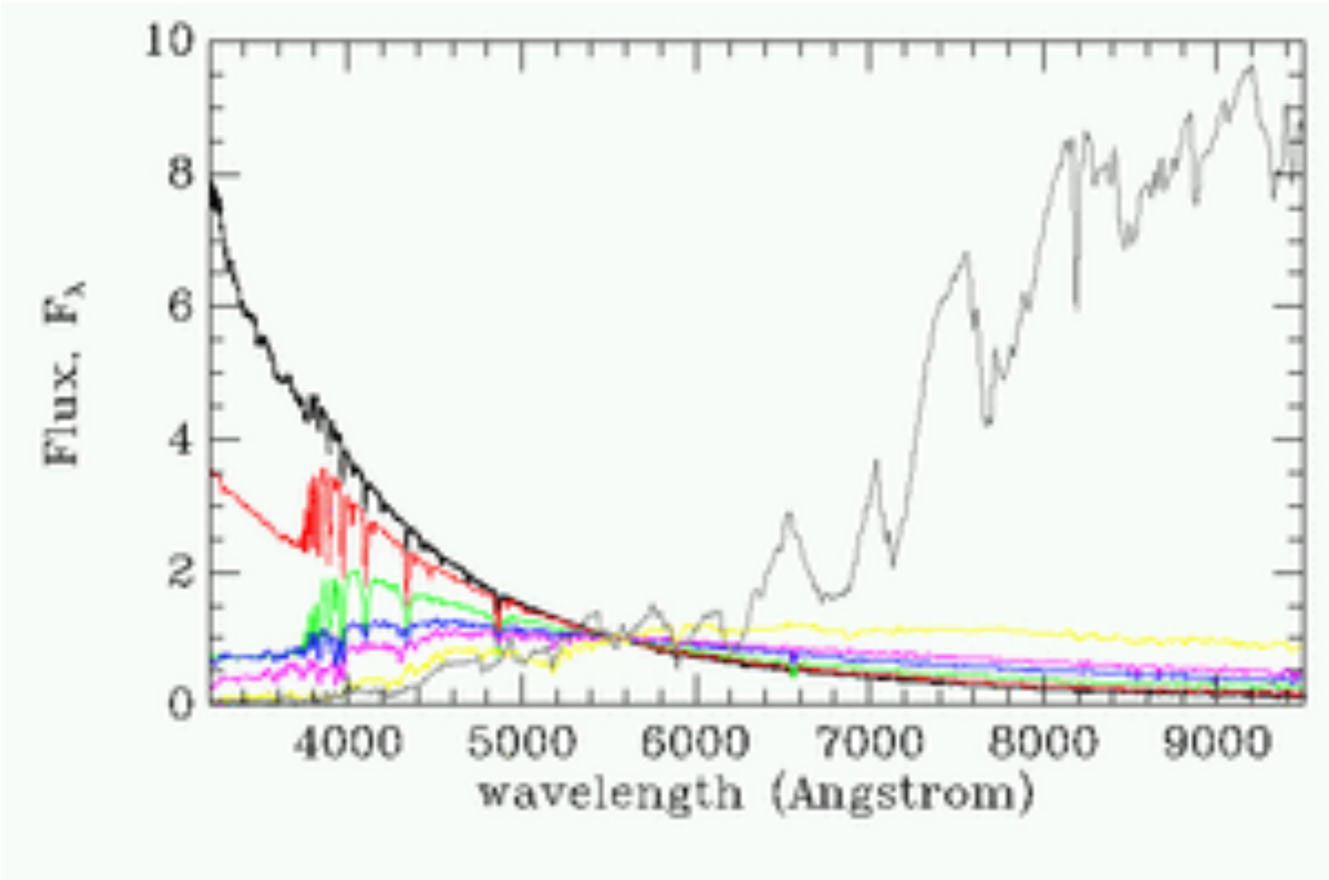
Summary of how to build a ML model and next steps

1. Choose a class of model (aka a machine learning algorithm) by importing the appropriate estimator class from Scikit-Learn.
2. Choose model hyperparameters by instantiating this class with desired values. Alternatively: optimize hyperparameters (later).
3. Arrange data into a features matrix and target vector, if necessary.
4. Split the learning set into training/test using k fold cross validation.
5. Fit the model to your data by calling the ``fit()`` method.
6. Apply the Model to new data: predict labels for unknown data using the ``predict()`` method.
7. Estimate the performance (averaged over the k folds) by using one of the metrics in the "metrics" method of the model instance (accuracy, precision, recall … or custom).
8. Figure out what is not working out: Check training vs test score, learning curves, diagnose high variance vs high bias and decide how to move forward.

Coding exercise: supervised classification problem, in which we are trying to decide if a star is a variable star (RR Lyrae), based on imaging data in 5 bands (u, g, r, i, z) and four colors (u-g, g-r, r-i, i-z)



range of observed brightness



spectra of different stellar types