Bias/Variance Dilemma

Lecture notes by Ethem Alpaydın
Introduction to Machine Learning (Boğaziçi Üniversitesi)

Lecture notes by Kevyn Collins-Thompson
Applied Machine Learning (Coursera)

Lecture notes by Andrew NG
Machine Learning by Stanford University (Coursera)

Model Selection & Generalization

- How well a model trained on the training set predicts the right output for new generalization instances is called *generalization*.
- Overfitting: $\mathcal{H}$ is more complex than the function
- Underfitting: $\mathcal{H}$ is less complex than the function

Triple Trade-Off

- In all learning algorithms that are trained from example data, there is a trade-off between three factors:
  - the complexity of the hypothesis we fit to data, namely, the capacity of the hypothesis class,
  - the amount of training data, and
  - the generalization error on new examples.

Triple Trade-Off

- As the complexity of the model class H increases, the generalization error decreases first and then starts to increase.
- As the amount of training data increases, the generalization error decreases.

Bias/Variance Dilemma

- Whenever we discuss model prediction, it's important to understand prediction errors (bias and variance).
- There is a tradeoff between a model's ability to minimize bias and variance.
- Gaining a proper understanding of these errors would help us not only to build accurate models but also to avoid the mistake of overfitting and underfitting.

https://towardsdatascience.com/understanding-the-bias-variance-tradeoff-165e6942b229

Bias/Variance Dilemma

- ***Bias*** is the difference between the average prediction of our model and the correct value which we are trying to predict.
- Model with *high bias* pays very little attention to the training data and oversimplifies the model.
- It always leads to high error on training and test data.

https://towardsdatascience.com/understanding-the-bias-variance-tradeoff-165e6942b229

Bias/Variance Dilemma

- ***Variance*** is the variability of model prediction for a given data point or a value which tells us spread of our data.
- Model with *high variance* pays a lot of attention to training data and does not generalize on the data which it hasn't seen before.
- As a result, such models perform very well on training data but has high error rates on test data.

https://towardsdatascience.com/understanding-the-bias-variance-tradeoff-165e6942b229

Bias/Variance Dilemma

- In supervised learning, **underfitting** happens when a model unable to capture the underlying pattern of the data.
- These models usually have high bias and low variance.
- It happens when we have very less amount of data to build an accurate model or when we try to build a linear model with a nonlinear data.
- Also, these kind of models are very simple to capture the complex patterns in data like Linear and logistic regression.

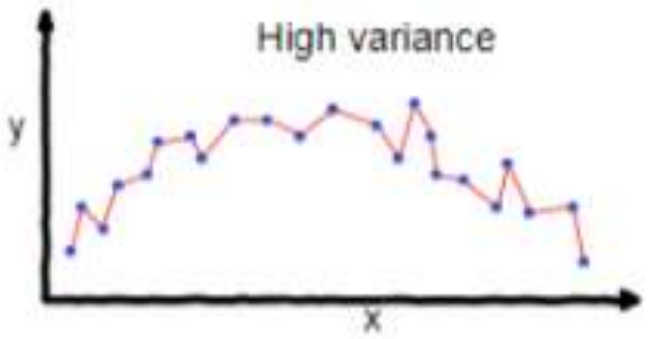
https://towardsdatascience.com/understanding-the-bias-variance-tradeoff-165e6942b229

Bias/Variance Dilemma

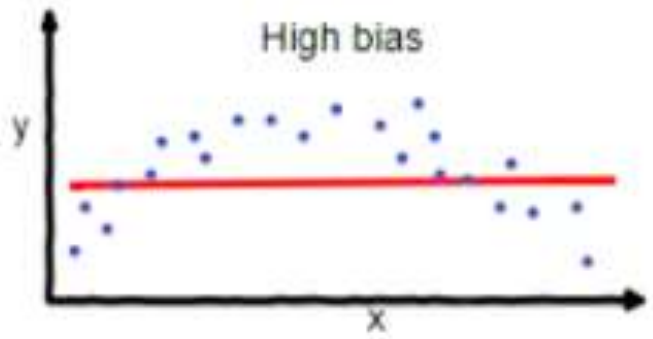
- In supervised learning, **overfitting** happens when our model captures the noise along with the underlying pattern in data.
- It happens when we train our model a lot over noisy dataset.
- These models have low bias and high variance.
- These models are very complex like Decision trees which are prone to overfitting.

https://towardsdatascience.com/understanding-the-bias-variance-tradeoff-165e6942b229

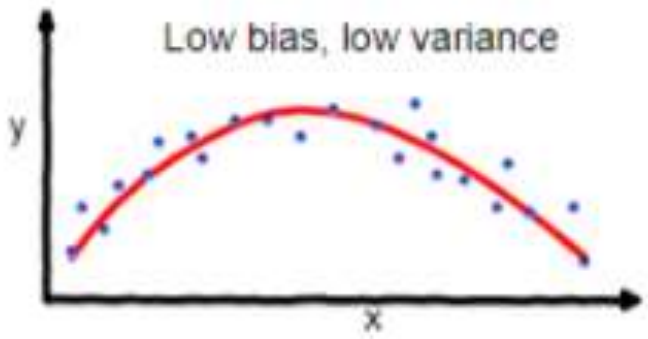
Bias/Variance Dilemma



overfitting



underfitting



Good balance

https://towardsdatascience.com/understanding-the-bias-variance-tradeoff-165e6942b229

Model Evaluation and Selection

Lecture notes by Ethem Alpaydın
Introduction to Machine Learning (Boğaziçi Üniversitesi)

Lecture notes by Kevyn Collins-Thompson
Applied Machine Learning (Coursera)

Data Mining: Concepts and Techniques, (3rd ed.)
Jiawei Han, Micheline Kamber, and Jian Pei

Lecture notes by Andrew NG
Machine Learning by Stanford University (Coursera)

Model Evaluation and Selection

- Evaluation metrics: How can we measure accuracy? Other metrics to consider?
- Use validation test set of class-labeled tuples instead of training set when assessing accuracy
- Methods for estimating a classifier's accuracy:
  - Holdout method, random subsampling
  - Cross-validation
  - Bootstrap
- Comparing classifiers:
  - Confidence intervals
  - Cost-benefit analysis and ROC Curves

Performance Metrics in Machine Learning

- Different performance metrics are used to evaluate different Machine Learning Algorithms.
- Important to choose the right metric when selecting between models and adjusting parameters.

Evaluation Metrics for Classification Problems

- Understand why accuracy only gives a partial picture of a classifier's performance.
- Understand the motivation and definition of important evaluation metrics in machine learning.
- Learn how to use a variety of evaluation metrics to evaluate supervised machine learning models.
- Learn about choosing the right metric for selecting between models or for doing parameter tuning.

Confusion Matrix

- It is one of the most intuitive and easiest metrics used for finding the correctness and accuracy of the model.
- It is used for Classification problem where the output can be of two or more types of classes.

https://medium.com/thalus-ai/performance-metrics-for-classification-problems-in-machine-learning-part-i-b085d432082b

Confusion Matrix

- Binary Classification

	Predicted class	
True Class	Yes	No
Yes	TP: True Positive	FN: False Negative
No	FP: False Positive	TN: True Negative

Terms associated with Confusion matrix

- **True Positives (TP):** True positives are the cases when the actual class of the data point was 1 (True) and the predicted is also 1 (True)

- **True Negatives (TN):** True negatives are the cases when the actual class of the data point was 0 (False) and the predicted is also 0 (False)

https://medium.com/thalus-ai/performance-metrics-for-classification-problems-in-machine-learning-part-i-b085d432082b

Terms associated with Confusion matrix

- **False Positives (FP):** False positives are the cases when the actual class of the data point was 0 (False) and the predicted is 1 (True). False is because the model has predicted incorrectly and positive because the class predicted was a positive one. (1)

- **False Negatives (FN):** False negatives are the cases when the actual class of the data point was 1 (True) and the predicted is 0 (False). False is because the model has predicted incorrectly and negative because the class predicted was a negative one. (0)

https://medium.com/thalus-ai/performance-metrics-for-classification-problems-in-machine-learning-part-i-b085d432082b

When to minimise what?

- We know that there will be some error associated with every model that we use for predicting the true class of the target variable.
- This will result in False Positives and False Negatives
- There’s no hard rule that says what should be minimised in all the situations.
- It purely depends on the business needs and the context of the problem you are trying to solve.

https://medium.com/thalus-ai/performance-metrics-for-classification-problems-in-machine-learning-part-i-b085d432082b

When to minimise what?

Minimising False Negatives: Cancer detection problem

Let’s say in our cancer detection problem example, out of 100 people, only 5 people have cancer. In this case, we want to correctly classify all the cancerous patients as even a very BAD model(Predicting everyone as NON-Cancerous) will give us a 95% accuracy(will come to what accuracy is). But, in order to capture all cancer cases, we might end up making a classification when the person actually NOT having cancer is classified as Cancerous. This might be okay as it is less dangerous than NOT identifying/capturing a cancerous patient since we will anyway send the cancer cases for further examination and reports. But missing a cancer patient will be a huge mistake as no further examination will be done on them.

https://medium.com/thalus-ai/performance-metrics-for-classification-problems-in-machine-learning-part-i-b085d432082b

When to minimise what?

- **Minimising False Positives:** Email Spam Detection

Let’s say that you are expecting an important email like hearing back from a recruiter or awaiting an admit letter from a university. Let’s assign a label to the target variable and say,**1:** “Email is a spam” and **0:**”Email is not a spam”

Suppose the Model classifies that important email that you are desperately waiting for, as Spam(case of False positive). Now, in this situation, this is pretty bad than classifying a spam email as important or not spam since in that case, we can still go ahead and manually delete it and it’s not a pain if it happens once a while. So in case of Spam email classification, minimising False positives is more important than False Negatives

https://medium.com/thalus-ai/performance-metrics-for-classification-problems-in-machine-learning-part-i-b085d432082b

Confusion Matrix in scikit learn

	Predicted class	
True Class	Yes	No
Yes	TP: True Positive	FN: False Negative
No	FP: False Positive	TN: True Negative

```
from sklearn.metrics import confusion_matrix
confusion = confusion_matrix(y_test, pred_logreg)
print("Confusion matrix:\n{}".format(confusion))
```

Confusion Matrix

- Always look at the confusion matrix for your classifier.

True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
	Predicted negative	Predicted positive	$N = 450$

Accuracy

- Accuracy in classification problems is the number of correct predictions made by the model over all kinds predictions made
- Accuracy is the number of correct predictions (TP and TN) divided by the number of all samples

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN} = \frac{TP + TN}{N}$$

Accuracy

True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
			$N = 450$
	Predicted negative	Predicted positive	

$$Accuracy = \frac{TP + TN}{N} = \frac{26 + 400}{450} = 0{,}946$$

Accuracy

When to use Accuracy: Accuracy is a good measure when the target variable classes in the data are nearly balanced.

When NOT to use Accuracy: Accuracy should NEVER be used as a measure when the target variable classes in the data are a majority of one class.

https://medium.com/thalus-ai/performance-metrics-for-classification-problems-in-machine-learning-part-i-b085d432082b

Classification Error

$$Error = \frac{FP + FN}{TP + TN + FP + FN}$$

$$Error = \frac{7 + 17}{400 + 26 + 17 + 7} = 0.060$$

True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
	Predicted negative	Predicted positive	$N = 450$

Precision

Precision measures how many of the samples predicted as positive are actually positive:

$$Precision = \frac{TP}{TP + FP}$$

Precision is used as a performance metric when the goal is to limit the number of false positives

Known as positive predictive value

Precision

True negative	TN = 400	FP = 7	
True positive	FN = 17	TP = 26	
	Predicted negative	Predicted positive	$N = 450$

$$Precision = \frac{TP}{TP + FP} = \frac{26}{26 + 7} = 0.787$$

Recall

- Recall measures how many of the positive samples are captured by the positive predictions:

$$Recall = \frac{TP}{TP + FN}$$

- Recall is used as performance metric when we need to identify all positive samples; that is, when it is important to avoid false negatives.
- Known as *sensitivity, hit rate, true positive rate (TPR)*

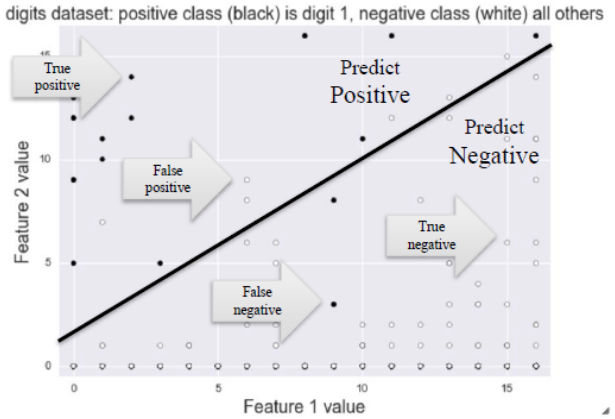
Tradeoff between precision and recall

Low Precision, High Recall

High Precision, Lower Recall

$$Precision = \frac{TP}{TP + FP}$$

$$Recall = \frac{TP}{TP + FN}$$



TN = 429	FP = 6
FN = 2	TP = 13

$$\text{Precision} = \frac{TP}{TP+FP} = \frac{13}{19} = 0.68$$

$$\text{Recall} = \frac{TP}{TP+FN} = \frac{13}{15} = 0.87$$

When to use Precision and When to use Recall?

It is clear that recall gives us information about a classifier's performance with respect to false negatives (how many did we miss), while precision gives us information about its performance with respect to false positives(how many did we caught).

Tradeoff between precision and recall

Recall-oriented machine learning tasks:

- Search and information extraction in legal discovery
- Tumor detection
- Often paired with a human expert to filter out false positives

Precision-oriented machine learning tasks:

- Search engine ranking, query suggestion
- Document classification
- Many customer-facing tasks (users remember failures!)

Tradeoff between precision and recall

While precision and recall are very important measures, looking at only one of them will not provide you with the full picture.

One way to summarize them is the *f-score* or *f-measure*, which is with the harmonic mean of precision and recall:

$$F = 2.\frac{precision\,.recall}{precision\ + recall}$$

Tradeoff between precision and recall

This particular variant is also known as the f_1-score.

As it takes precision and recall into account, it can be a better measure than accuracy on imbalanced binary classification datasets.

$$f_1 = 2.\frac{precision\,.recall}{precision\ + recall} = \frac{2.TP}{2.TP + FN + FP}$$

False Positive Rate

What fraction of all negative instances does the classifier incorrectly identify as positive?

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

known as *false alarm rate*

Sensitivity and Specificity

- **Sensitivity** is the same as true positive rate and recall

$$Sensitivity = \frac{TP}{TP + FN}$$

- **Specificity** is how well we detect the negatives, which is the number of true negatives divided by the total number of negatives; this is equal to 1 minus the false alarm rate

$$Specificity = 1 - FPR = 1 - \frac{FP}{TN + FP} = \frac{TN}{TN + FP}$$

Summary

	Predicted class		
True Class	Positive	Negative	Total
Positive	tp : true positive	fn : false negative	p
Negative	fp : false positive	tn : true negative	n
Total	p'	n'	N

Name	Formula
error	$(fp + fn)/N$
accuracy	$(tp + tn)/N = 1 - \text{error}$
tp-rate	tp/p
fp-rate	fp/n
precision	tp/p'
recall	$tp/p = \text{tp-rate}$
sensitivity	$tp/p = \text{tp-rate}$
specificity	$tn/n = 1 - \text{fp-rate}$

Scikit learn

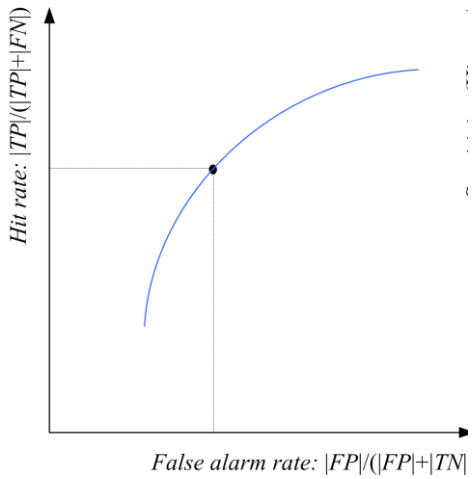
```
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score
# Accuracy = TP + TN / (TP + TN + FP + FN)
# Precision = TP / (TP + FP)
# Recall = TP / (TP + FN)  Also known as sensitivity, or True Positive Rate
# F1 = 2 * Precision * Recall / (Precision + Recall)
print('Accuracy: {:.2f}'.format(accuracy_score(y_test, tree_predicted)))
print('Precision: {:.2f}'.format(precision_score(y_test, tree_predicted)))
print('Recall: {:.2f}'.format(recall_score(y_test, tree_predicted)))
print('F1: {:.2f}'.format(f1_score(y_test, tree_predicted)))
```

ROC curve

An **ROC curve** (**receiver operating characteristic curve**) is a graph showing the performance of a classification model at all classification thresholds. This curve plots two parameters:

True Positive Rate $TPR = \frac{TP}{TP+FN}$

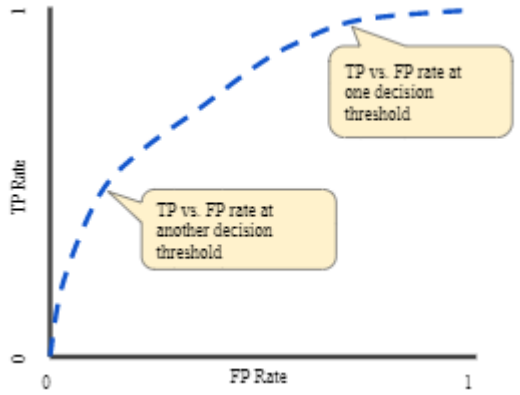
False Positive Rate $FPR = \frac{FP}{TN+FP}$



https://developers.google.com/machine-learning/crash-course/classification/roc-and-auc

ROC curve

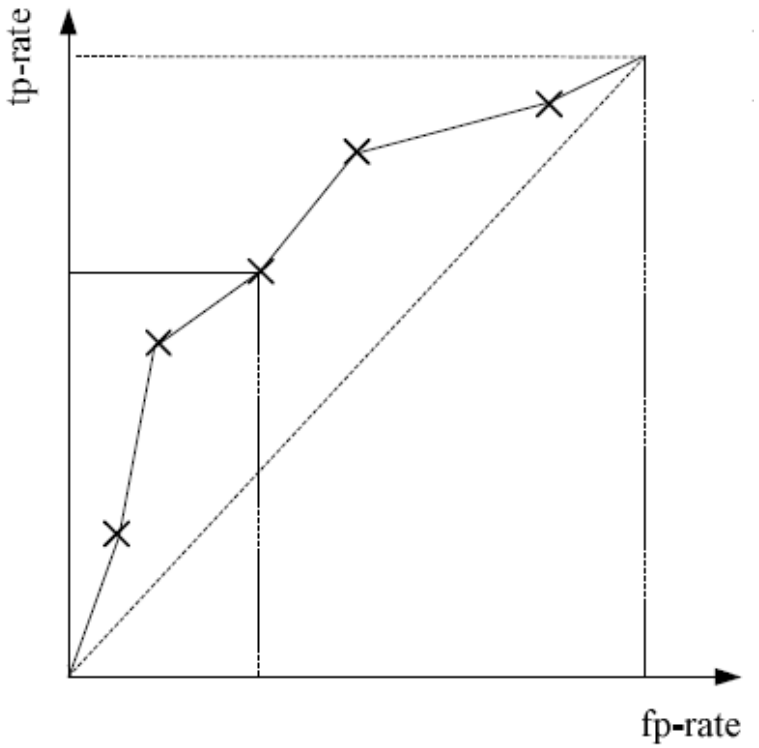
- An ROC curve plots TPR vs. FPR at different classification thresholds. Lowering the classification threshold classifies more items as positive, thus increasing both False Positives and True Positives.
- The following figure shows a typical ROC curve.



https://developers.google.com/machine-learning/crash-course/classification/roc-and-auc

ROC curve

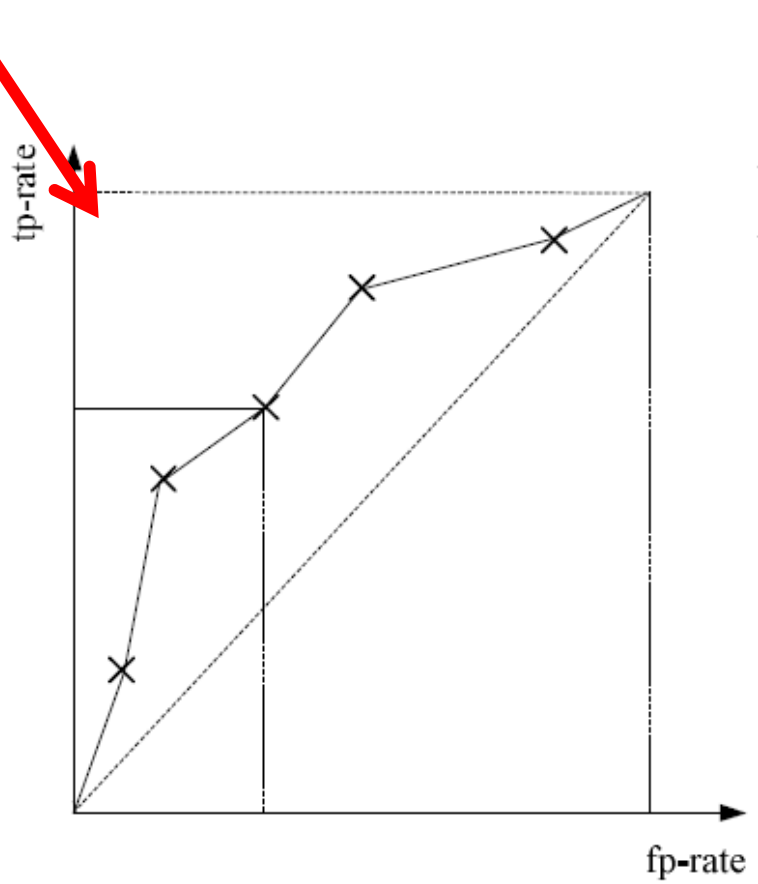
Each classifier has a threshold that allows us to move over this curve, and we decide on a point, based on the relative importance of hits versus false alarms, namely, true positives and false positives.



(a) Example ROC curve

ROC curve

- Ideally, a classifier has a tp-rate of 1 and a fp-rate of 0, and hence a classifier is better the more it gets closer to the upper-left corner



(a) Example ROC curve

Area Under the Curve (AUC)

- ROC is a probability curve and AUC represents degree or measure of separability.
- It tells how much model is capable of distinguishing between classes.
- Higher the AUC, better the model is at predicting 0s as 0s and 1s as 1s

https://towardsdatascience.com/understanding-auc-roc-curve-68b2303cc9c5

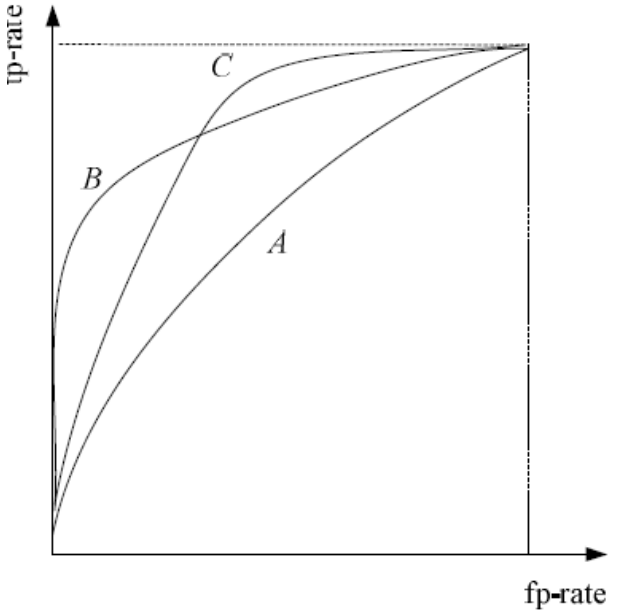
Area Under the Curve (AUC)

Summarizing an ROC curve in one number: Area Under the Curve (AUC)

A classifier ideally has an AUC of 1 and AUC values of different classifiers can be compared to give us a general performance averaged over different loss conditions.

AUC = 0 (worst) AUC = 1 (best)

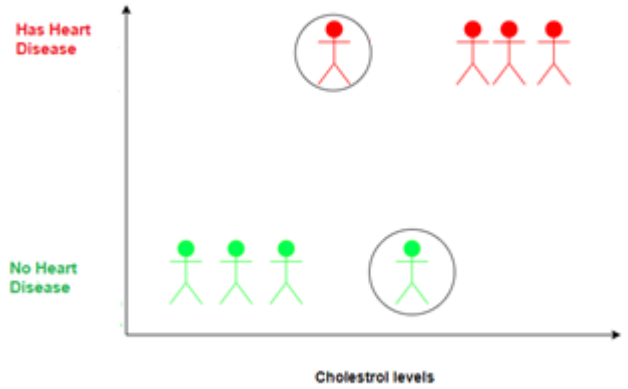
B and C are preferred over A



(b) Different ROC curves for different classifiers

ROC Curve - example

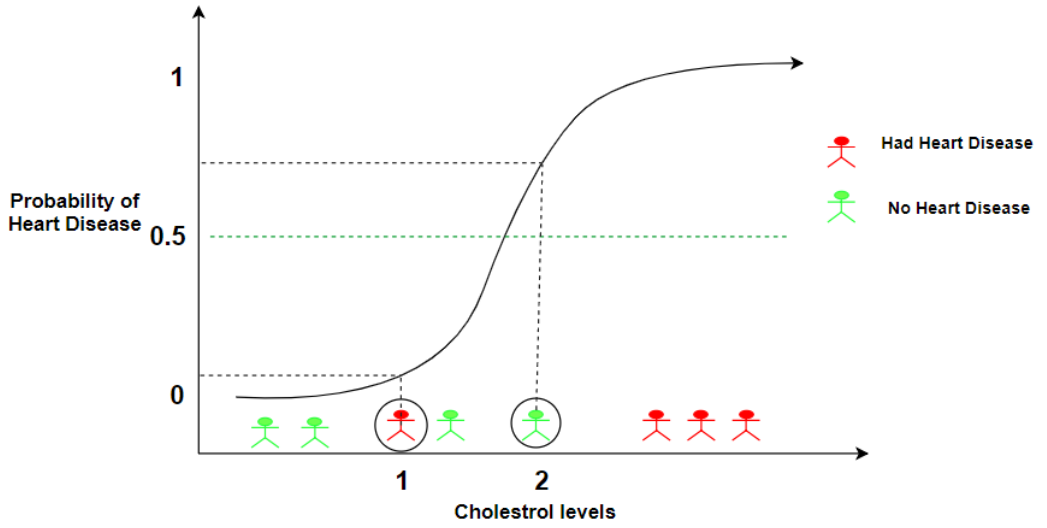
- Consider a **hypothetical example** containing a group of people.
- The y-axis has two categories i.e **Has Heart Disease** represented by red people and **does not have Heart Disease** represented by green circles.
- **A** long the x-axis, we have **cholesterol** levels and the classifier tries to classify people into two categories depending upon their cholesterol levels



https://towardsdatascience.com/understanding-the-roc-and-auc-curves-a05b68550b69

ROC Curve - example

- Let us now evaluate the effectiveness of logistic regression with the classification threshold set to 0.5, with some new people about whom we already know if they have heart disease or not.



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ROC Curve - example

- Let’s create a Confusion Matrix to summarize the classifications

		Actual	
		Has Heart Disease	Doesnot have Heart Disease
Predicted	Has Heart Disease	3	1
	Doesnot have Heart Disease	1	3

- Once the confusion matrix is filled in, we can calculate the True Positive rate and the False Positive Rate to evaluate this logistic regression at 0.5 threshold.

https://towardsdatascience.com/understanding-the-roc-and-auc-curves-a05b68550b69

ROC Curve - example

True Positive Rate $TPR = \frac{TP}{TP+FN} = \frac{3}{4} = 0.75$

False Positive Rate $FPR = \frac{FP}{TN+FP} = \frac{1}{1+3} = 0.25$

		Actual	
		Has Heart Disease	Doesnot have Heart Disease
Predicted	Has Heart Disease	3	1
	Doesnot have Heart Disease	1	3

https://towardsdatascience.com/understanding-the-roc-and-auc-curves-a05b68550b69

ROC Curve - example

Let’s talk about what happens when we use a different threshold for deciding if a person has heart disease or not

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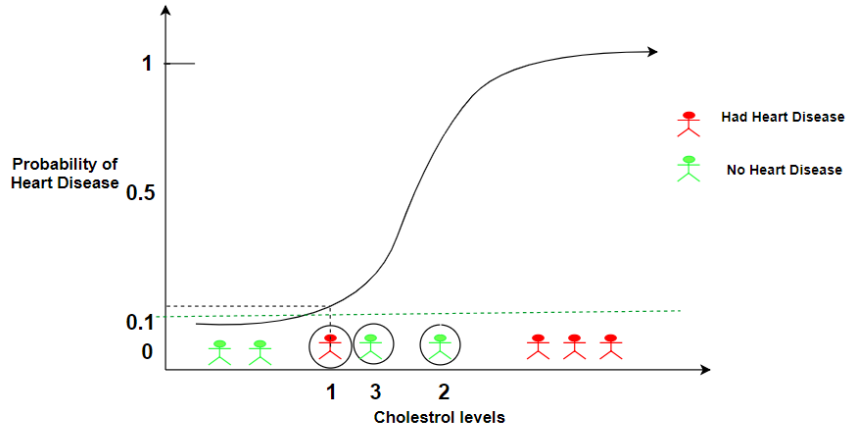
ROC Curve - example

Setting the Threshold to 0.1



		Actual: Has Heart Disease	Actual: Doesnot have Heart Disease
Predicted	Has Heart Disease	4	2
	Doesnot have Heart Disease	0	2

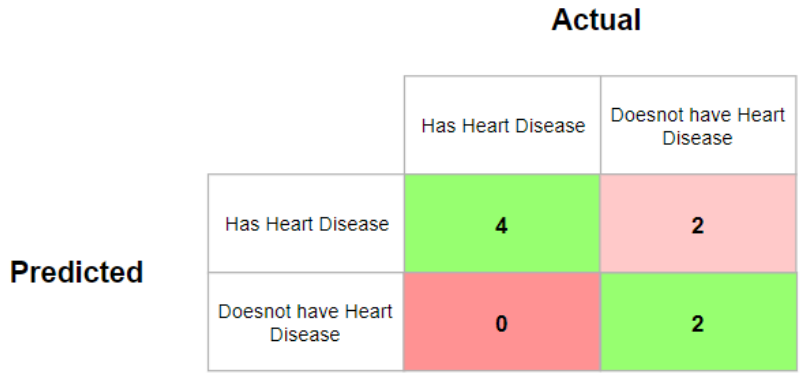
a lower threshold:
Increases the number of False Positives
Decreases the number of False Negatives

https://towardsdatascience.com/understanding-the-roc-and-auc-curves-a05b68550b69

ROC Curve - example

True Positive Rate $TPR = \frac{TP}{TP+FN} = \frac{4}{4+0} = 1$

False Positive Rate $FPR = \frac{FP}{TN+FP} = \frac{2}{2+2} = 0.5$



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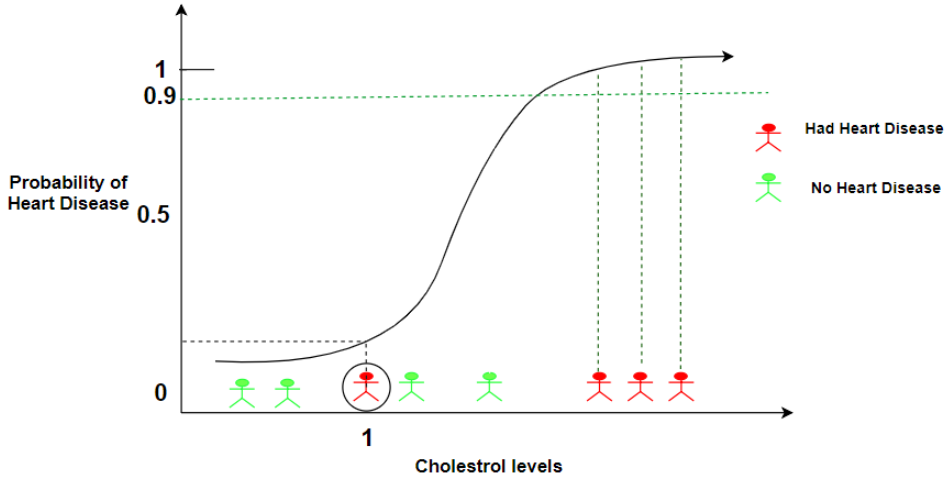
ROC Curve - example

Setting the Threshold to 0.9



Actual

	Has Heart Disease	Doesnot have Heart Disease
Has Heart Disease	**3**	**0**
Doesnot have Heart Disease	**1**	**4**

a higher threshold:
Decreases the number of False Positives
Increases the number of False Negatives

https://towardsdatascience.com/understanding-the-roc-and-auc-curves-a05b68550b69

ROC Curve - example

True Positive Rate $TPR = \frac{TP}{TP+FN} = \frac{3}{3+1} = 0.75$

False Positive Rate $FPR = \frac{FP}{TN+FP} = \frac{0}{4+0} = 0$

		Actual
	Has Heart Disease	Doesnot have Heart Disease
Has Heart Disease	**3**	**0**
Doesnot have Heart Disease	**1**	**4**

https://towardsdatascience.com/understanding-the-roc-and-auc-curves-a05b68550b69

ROC Curve - example

Thresholds

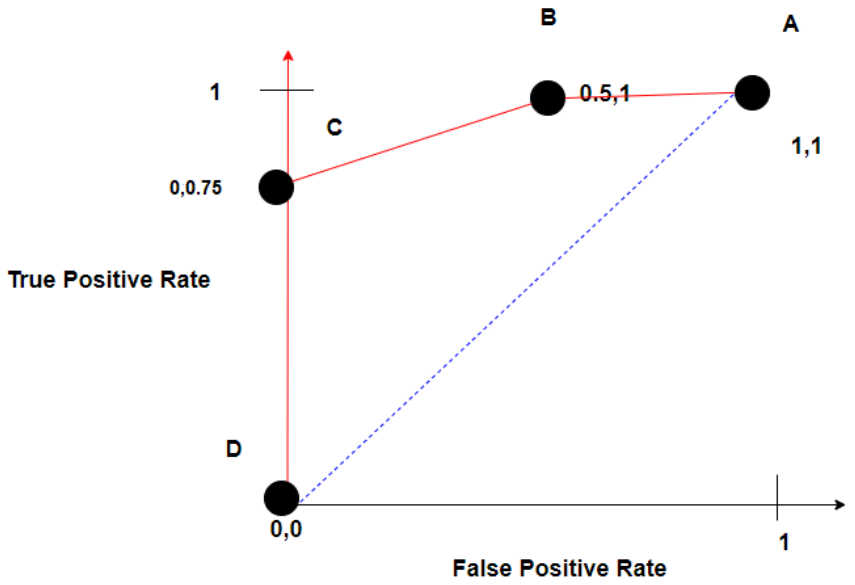
A=0

B=0.1

C=0.9

D=1

$$A < B < C < D$$



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Metrics for Multiclass Classification

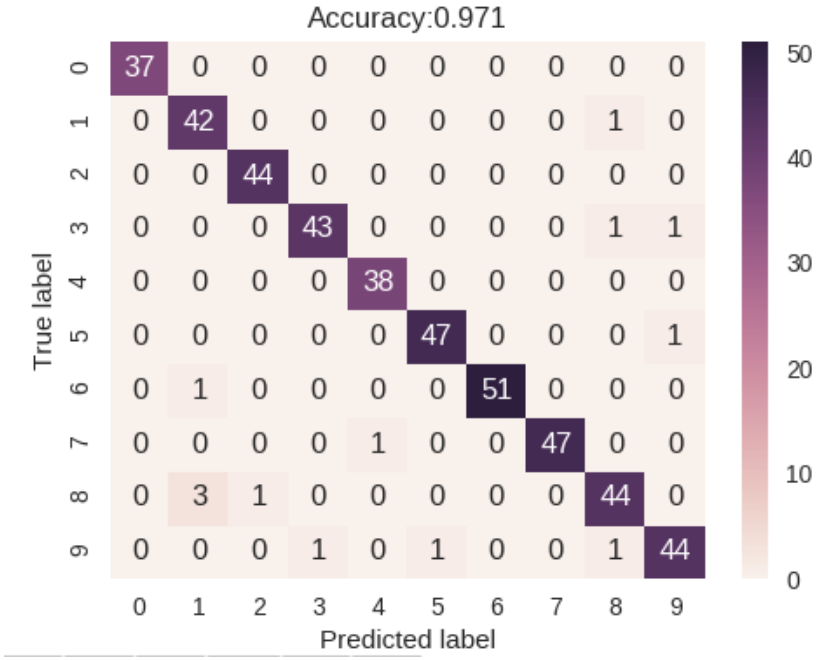
Multi-class evaluation is an extension of the binary case.

- A collection of true vs predicted binary outcomes, one per class
- Confusion matrices are especially useful
- Classification report

- Accuracy for multiclass classification is again defined as the fraction of correctly classified examples.

Metrics for Multiclass Classification

Confusion matrix for the 10-digit classification task



$$Accuracy = \frac{\sum_i diag_i}{N}$$

Metrics - example

Confusion matrix

	a_B	a_P	a_S	a_T	a_H
p_B	17	3	2	3	2
p_P	1	12	0	1	2
p_S	0	1	16	0	1
p_T	3	3	1	13	1
p_H	0	0	0	0	16

	a_B	a_P	a_S	a_T	a_H
p_B				fn	
p_P				fn	
p_S				fn	
p_T	fp	fp	fp	tp	fp
p_H				fn	

$$Precision_X = \frac{TP_X}{TP_x + FP_X} = \frac{TP_x}{TotalPredicted_X} \rightarrow \quad Precision_T = \frac{13}{13+3+3+1+1} = 0.62$$

$$Recall_X = \frac{TP_X}{TP_x + FN_x} = \frac{TP_x}{TotalClass_X} \rightarrow Recall_T = \frac{13}{13+3+1} = 0.76$$

Metrics - example

	GoldLabel_A	GoldLabel_B	GoldLabel_C	
Predicted_A	**30**	20	10	TotalPredicted_A=60
Predicted_B	50	**60**	10	TotalPredicted_B=120
Predicted_C	20	20	**80**	TotalPredicted_C=120
	TotalGoldLabel_A=100	TotalGoldLabel_B=100	TotalGoldLabel_C=100	

$$Precision_X = \frac{TP_X}{TP_x + FP_X} \rightarrow \quad Precision_A = \frac{30}{30 + 20 + 10} = 0.5$$

$$Recall_X = \frac{TP_X}{TP_x + FN_x} \rightarrow Recall_A = \frac{30}{30 + 50 + 20} = 0.3$$

Scikit learn

In[65]:

```
print(classification_report(y_test, pred))
```

Out[65]:

	precision	recall	f1-score	support
0	1.00	1.00	1.00	37
1	0.89	0.91	0.90	43
2	0.95	0.93	0.94	44
3	0.90	0.96	0.92	45
4	0.97	1.00	0.99	38
5	0.98	0.98	0.98	48
6	0.96	1.00	0.98	52
7	1.00	0.94	0.97	48
8	0.93	0.90	0.91	48
9	0.96	0.94	0.95	47
avg / total	0.95	0.95	0.95	450

Micro vs Macro Average

- "macro" averaging computes the unweighted per-class *f*-scores. This gives equal weight to all classes, no matter what their size is.
- "micro" averaging computes the total number of false positives, false negatives, and true positives over all classes, and then computes precision, recall, and *f*-score using these counts.

Micro vs Macro Average

Class	Predicted Class	Correct?
orange	lemon	0
orange	lemon	0
orange	apple	0
orange	orange	1
orange	apple	0
lemon	lemon	1
lemon	apple	0
apple	apple	1
apple	apple	1

Macro-average:

- Each class has equal weight.

1. Compute metric within each class
2. Average resulting metrics across classes

Class	Recall
orange	1/5 = 0.20
lemon	1/2 = 0.50
apple	2/2 = 1.00

Macro-average
(0.20 + 0.50 + 1.00) / 3 = **0.57**

Micro vs Macro Average

Class	Predicted Class	Correct?
orange	lemon	0
orange	lemon	0
orange	apple	0
orange	orange	1
orange	apple	0
lemon	lemon	1
lemon	apple	0
apple	apple	1
apple	apple	1

Micro-average:

- Each instance has equal weight.
- Largest classes have most influence

1. Aggregrate outcomes across all classes
2. Compute metric with aggregate outcomes

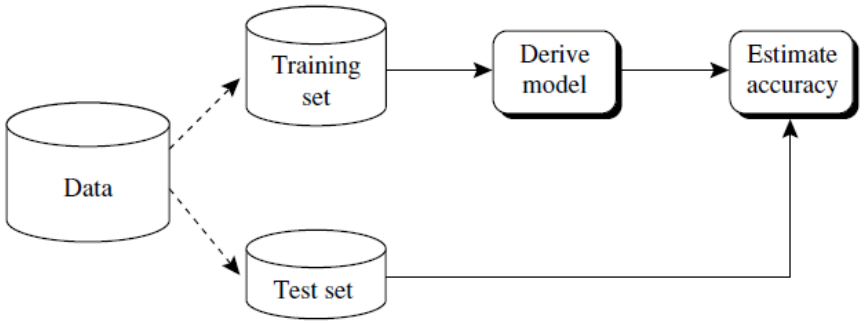
Micro-average precision:
4 / 9 = **0.44**

Evaluating Classifier Accuracy

- Holdout
- Cross validation
- Bootstrap

Holdout

- Given data is randomly partitioned into two independent sets
  - Training set (e.g., 2/3) for model construction
  - Test set (e.g., 1/3) for accuracy estimation
- Random sampling: a variation of holdout
  - Repeat holdout k times, accuracy = avg. of the accuracies obtained



Estimating accuracy with the holdout method.

Cross-Validation

- *Cross-validation* is a statistical method of evaluating generalization performance that is more stable and thorough than using a split into a training and a test set.
- In cross-validation, the data is instead split repeatedly and multiple models are trained.

K-fold cross-validation

- The most commonly used version of cross-validation is *k-fold cross-validation*, where *k* is a user-specified number, usually 5 or 10.

K-fold cross-validation

- The need for multiple training/validation sets $\{X_i,V_i\}_i$:

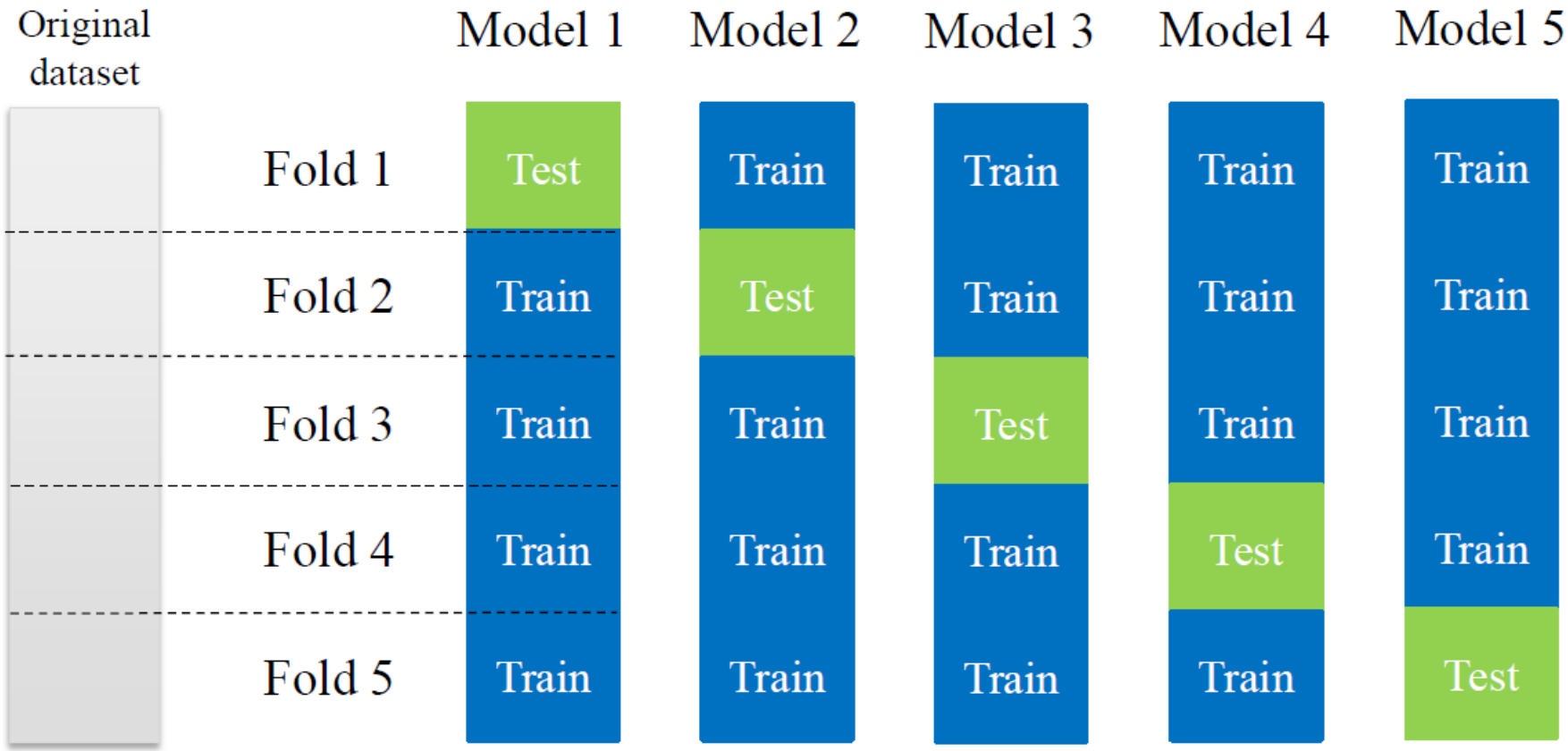
  Training/validation sets of fold *i*

- *K*-fold cross-validation: Divide X into *k*, X_i,*i*=1,...,*K*

$$\mathcal{V}_1 = \mathcal{X}_1 \quad \mathcal{T}_1 = \mathcal{X}_2 \cup \mathcal{X}_3 \cup \cdots \cup \mathcal{X}_K$$
$$\mathcal{V}_2 = \mathcal{X}_2 \quad \mathcal{T}_2 = \mathcal{X}_1 \cup \mathcal{X}_3 \cup \cdots \cup \mathcal{X}_K$$
$$\vdots$$
$$\mathcal{V}_K = \mathcal{X}_K \quad \mathcal{T}_K = \mathcal{X}_1 \cup \mathcal{X}_2 \cup \cdots \cup \mathcal{X}_{K-1}$$

- T_i share *K*-2 parts

K-fold cross-validation



Cross-Validation in scikit-learn

- Cross-validation is implemented in scikit-learn using the `cross_val_score` function from the `model_selection` module.
- The parameters of the `cross_val_score` function are the model we want to evaluate, the training data, and the ground-truth labels

Cross-Validation in scikit-learn

Let’s evaluate LogisticRegression on the iris dataset

```
from sklearn.model_selection import cross_val_score
from sklearn.datasets import load_iris
from sklearn.linear_model import LogisticRegression
iris = load_iris()
logreg = LogisticRegression()
scores = cross_val_score(logreg, iris.data, iris.target)
print("Cross-validation scores: {}".format(scores))
```

Cross-Validation in scikit-learn

- By default, `cross_val_score` performs three-fold cross-validation, returning three accuracy values

Output:

Cross-validation scores: [0.961 0.922 0.958]

Cross-Validation in scikit-learn

We can change the number of folds used by changing the `cv` parameter:

```
scores = cross_val_score(logreg, iris.data, iris.target, cv=5)
print("Cross-validation scores: {}".format(scores))
```

Output:

Cross-validation scores: [1. 0.967 0.933 0.9 1.]

Cross-Validation in scikit-learn

A common way to summarize the cross-validation accuracy is to compute the mean:

```
print("Average cross-validation score: {:.2f}".format(scores.mean()))
```

Output:

Average cross-validation score: 0.96

Benefits of Cross-Validation

- When using cross-validation, each example will be in the training set exactly once: each example is in one of the folds, and each fold is the validation set once.
- Therefore, the model needs to generalize well to all of the samples in the dataset for all of the cross-validation scores (and their mean) to be high
- Having multiple splits of the data also provides some information about how sensitive our model is to the selection of the training dataset.
- Another benefit of cross-validation as compared to using a single split of the data is that we use our data more effectively.

Disadvantage of cross-validation

- The main disadvantage of cross-validation is increased computational cost.
  - As we are now training *k* models instead of a single model, cross-validation will be roughly *k* times slower than doing a single split of the data.

Stratified Cross-validation

- Splitting the dataset into *k* folds by starting with the first one-*k*-th part of the data might not always be a good idea

Stratified Cross-validation

fruit_label	fruit_name
1	Apple
1	Apple
1	Apple
1	Apple
1	Apple
2	Mandarin
...	...
3	Orange
...	...
4	Lemon
4	Lemon
4	Lemon
4	Lemon
4	Lemon

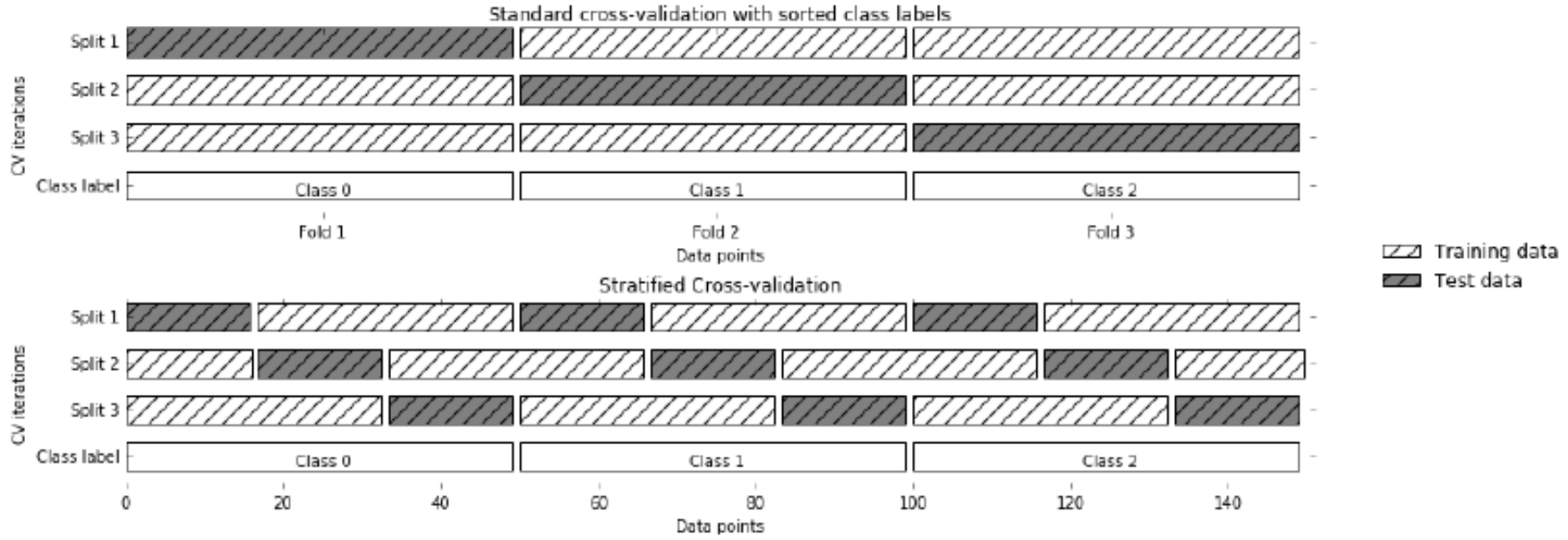
Example has 20 data samples = 4 classes with 5 samples each.

5-fold CV: 5 folds of 4 samples each.

Fold 1 uses the first 20% of the dataset as the test set, which only contains samples from class 1.

Classes 2, 3, 4 are missing entirely from test set and so will be missing from the evaluation.

Stratified Cross-validation

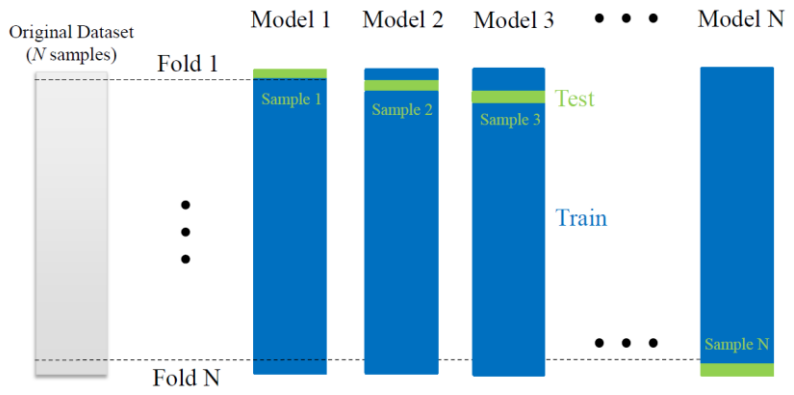


Stratified Cross-validation

- For example, if 90% of your samples belong to class A and 10% of your samples belong to class B, then stratified cross-validation ensures that in each fold, 90% of samples belong to class A and 10% of samples belong to class B.

Leave-one-out

- Each fold is a single sample.
- This can be very time consuming, particularly for large datasets, but sometimes provides better estimates on small datasets
- This is typically used in applications such as medical diagnosis, where labeled data is hard to find



Leave-one-out in scikit-learn

```
from sklearn.model_selection import LeaveOneOut
loo = LeaveOneOut()
scores = cross_val_score(logreg, iris.data, iris.target, cv=loo)
print("Number of cv iterations: ", len(scores))
print("Mean accuracy: {:.2f}".format(scores.mean()))
```

Output:

Number of cv iterations: 150

Mean accuracy: 0.95

Bootstrapping

- To generate multiple samples from a single sample, an alternative to cross-validation is the *bootstrap* that generates new samples by drawing instances from the original sample *with* replacement.
- The bootstrap samples may overlap more than cross-validation samples and hence their estimates are more dependent; but is considered the best way to do resampling for very small datasets.

Bootstrapping

- In the bootstrap, we sample *N* instances from a dataset of size *N* with replacement.
- The original dataset is used as the validation set.
- The probability that we pick an instance is 1*/N*; the probability that we do not pick it is 1 − 1*/N*
- Prob that we do not pick an instance after N draws

$$\left(1-\frac{1}{N}\right)^{N} \approx e^{-1} = 0.368$$

that is, only 36.8% is new!

Model Selection

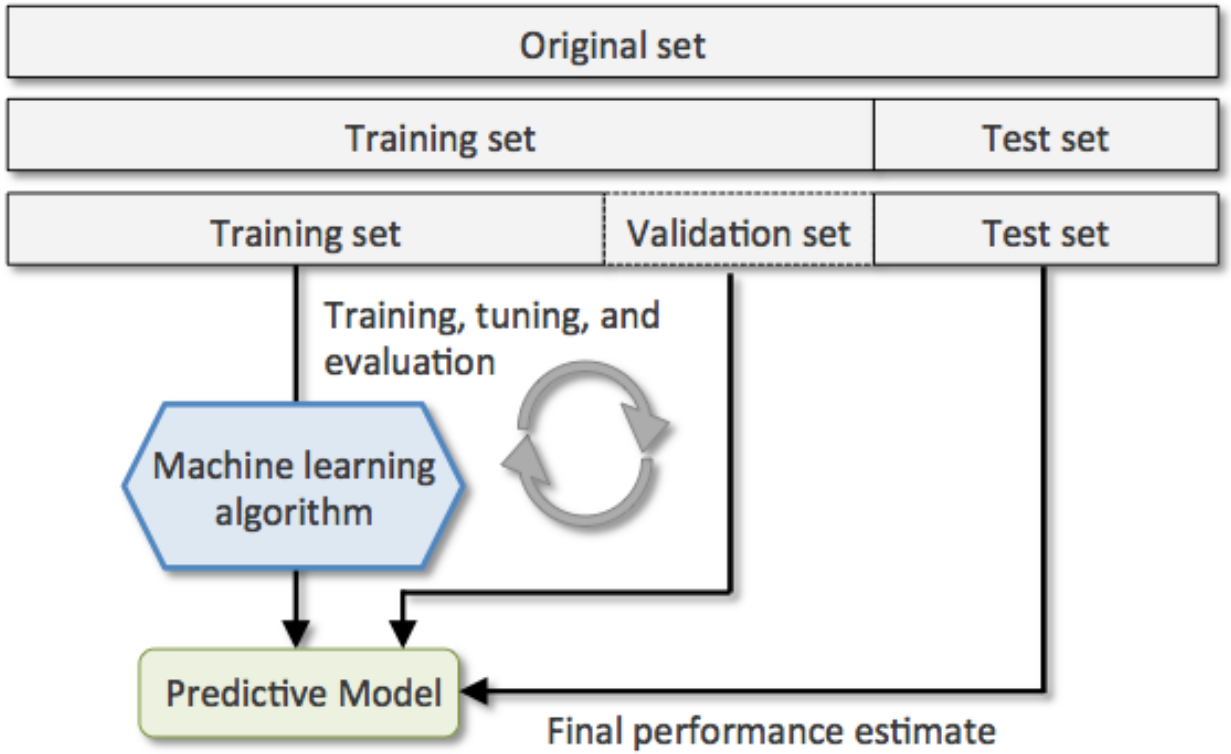
1. Split data
   - Training set (model building)
   - Validation set (model selection)
   - Test set (final evaluation)
2. Learn parameter from training data (minimizing traning error)
3. Compute cross validation set error.
4. Select the model with lowest cross validation set error.
5. Estimate generalization error for test set

Train / Validation / Test Data

	Purpose	Yield	Used for Model training	Used for Parameter tuning
Train Data	To learn patterns from the data.	A model that makes near-expected predictions	Yes	Yes
Validation Data	To understand model behaviour and generalizibility on unseen data.	Insights on how to tune your model.	No	Yes
Test Data	To understand how the model would perform in real world scenario.	A completely unbiased estimate of model performance.	No	No

https://medium.com/datadriveninvestor/data-science-essentials-why-train-validation-test-data-b7f7d472dc1f

Train / Validation / Test Data



https://medium.com/datadriveninvestor/data-science-essentials-why-train-validation-test-data-b7f7d472dc1f

Model Selection

- Now that we know how to evaluate how well a model generalizes, we can take the next step and improve the model's generalization performance by tuning its parameters.
- The most commonly used method is *grid search*, which basically means trying all possible combinations of the parameters of interest.

Grid Search: Example

Consider the case of a kernel SVM with an RBF (radial basis function) kernel, as implemented in the SVC class.

- There are two important parameters: the kernel bandwidth, gamma, and the regularization parameter, C.
- Say we want to try the values 0.001, 0.01, 0.1, 1, 10, and 100 for the parameter C, and the same for gamma.
- Because we have six different settings for C and gamma that we want to try, we have 36 combinations of parameters in total

Grid Search in scikit-learn

Because grid search with cross-validation is such a commonly used method to adjust parameters, scikit-learn provides the `GridSearchCV` class, which implements it in the form of an estimator.

Grid Search in scikit-learn

```
param_grid = {'C': [0.001, 0.01, 0.1, 1, 10, 100],
               'gamma': [0.001, 0.01, 0.1, 1, 10, 100]}
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC
grid_search = GridSearchCV(SVC(), param_grid, cv=5)
X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target, random_state=0)
grid_search.fit(X_train, y_train)
print("Test set score: {:.2f}".format(grid_search.score(X_test, y_test)))
print("Best parameters: {}".format(grid_search.best_params_))
print("Best cross-validation score: {:.2f}".format(grid_search.best_score_))
print("Best estimator:\n{}".format(grid_search.best_estimator_))
```