EVML3

ML PERFORMANCE

JEROEN VEEN

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OF APPLIED SCIENCES

QUIZ TIME

- Individual, multiple-choice questions
- Online: http://www.socrative.com room **1PTGB6PY**
- Open book quiz, so books and slides can be consulted

- **HAN student number**, so NOT your name, nickname or anything else.
- Quiz starts exactly at class hour and takes 10 minutes.
- Be on time and have your equipment prepared.

CONTENTS

- Confusion matrix
- Evaluating classifiers
- Learning curves

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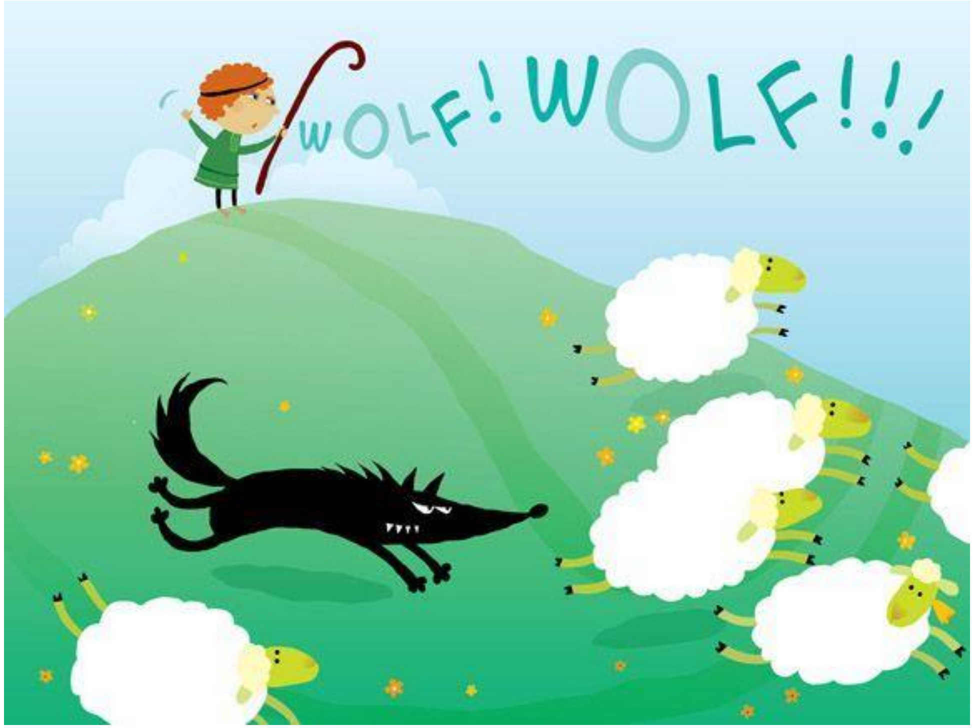
VEROS COVID-19
DELIVERED:1
Accuracy 97.9%
Sensitivity 95.2%
Specificity 99.5%
CONTROL
COVID-19
veros™
COVID-19

THE BOY WHO CRIED WOLF

"Wolf" is a **positive class**.

"No wolf" is a **negative class**

An Aesop's Fable ~620 BCE



Source: Sam Taplin

CONFUSION MATRIX

ACTUAL

(Type I error)

PREDICTED		
	True Positive (TP) Reality: A wolf threatened. Shepherd said: "Wolf." Outcome: Shepherd is a hero.	**False Positive (FP)** Reality: No wolf threatened. Shepherd said: "Wolf." Outcome: Villagers are angry at shepherd for waking them up.
	False Negative (FN) Reality: A wolf threatened. Shepherd said: "No wolf." Outcome: The wolf ate all the sheep.	**True Negative (TN)** Reality: No wolf threatened. Shepherd said: "No wolf." Outcome: Everyone is fine.

Type II error)

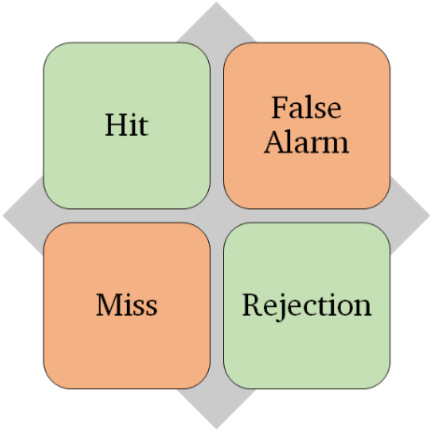
ACCURACY

- Fraction of predictions the model got right

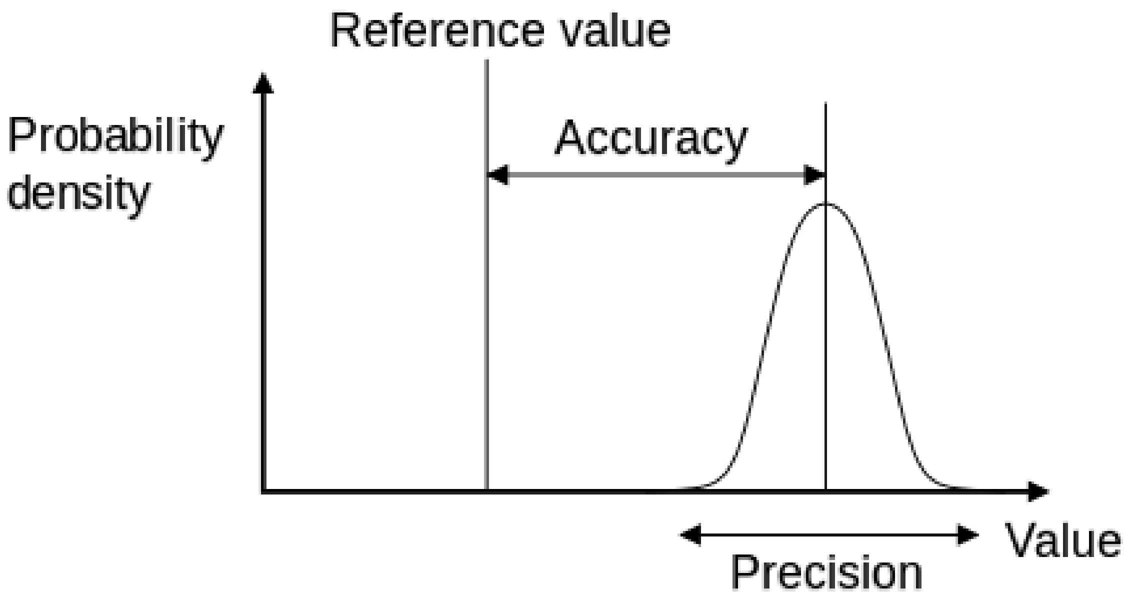
$$\text{Accuracy} = \frac{\text{Number of correct predictions}}{\text{Total number of predictions}}$$

- For binary classification

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



ACCURACY VS PRECISION



accuracy is closeness of the measurements to a specific value, while **precision** is the closeness of the measurements to each other.

Source: https://en.wikipedia.org/wiki/Accuracy_and_precision

PRECISION AND RECALL

- Precision, fraction of correct positive predictions

  Σ True positive / Σ Predicted condition positive

$$\text{precision} = \frac{TP}{TP + FP}$$

- Recall, probability of detection

  Σ True positive / Σ Condition positive

$$\text{recall} = \frac{TP}{TP + FN}$$

precision

recall

True Positive (TP) Reality: A wolf threatened. Shepherd said: "Wolf." Outcome: Shepherd is a hero.	**False Positive (FP)** Reality: No wolf threatened. Shepherd said: "Wolf." Outcome: Villagers are angry at shepherd for waking them up.
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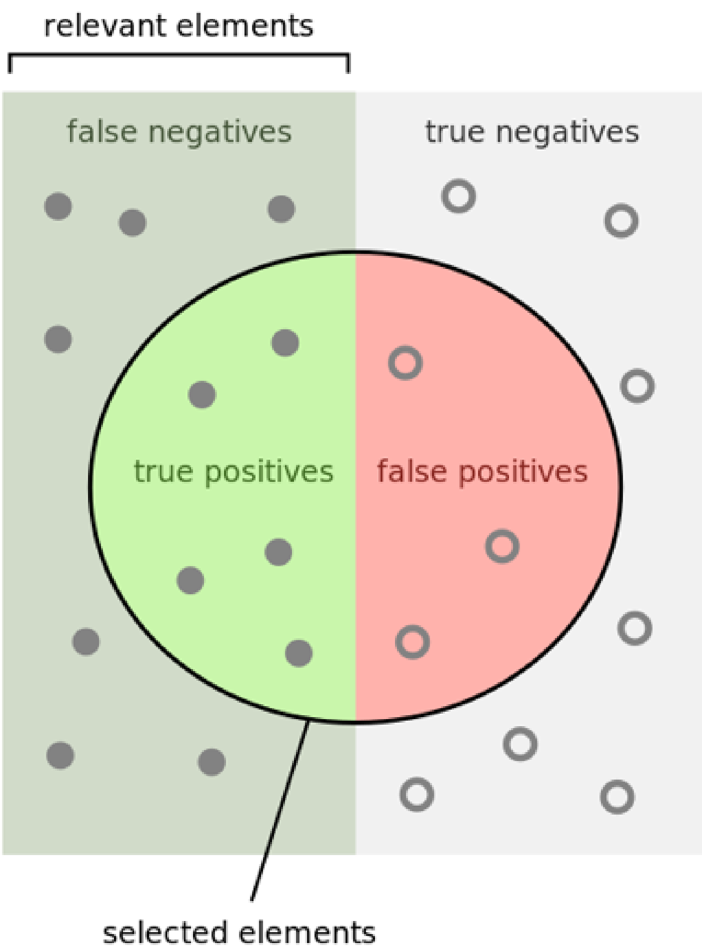
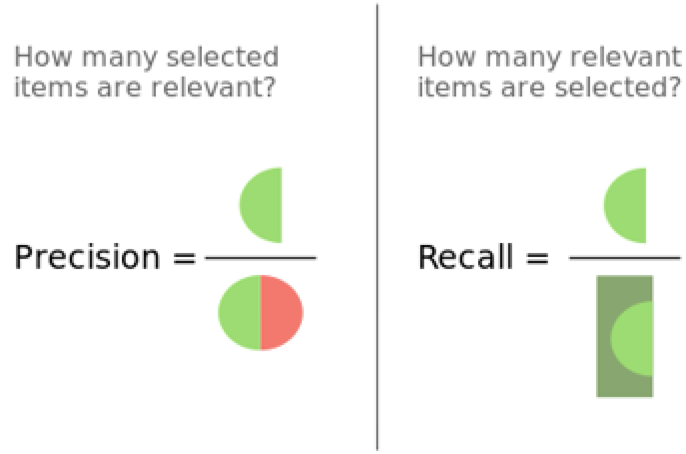
PRECISION AND RECALL





Recall = sensitivity = true positive rate (TPR)

Source: https://en.wikipedia.org/wiki/Precision_and_recall

SKLEARN CLASSIFICATION REPORT

.

```
>>> from sklearn.metrics import classification_report
>>> y_true = [0, 1, 2, 2, 2]
>>> y_pred = [0, 0, 2, 2, 1]
>>> target_names = ['class 0', 'class 1', 'class 2']
>>> print(classification_report(y_true, y_pred, target_names=target_names))
              precision    recall  f1-score   support

     class 0       0.50      1.00      0.67         1
     class 1       0.00      0.00      0.00         1
     class 2       1.00      0.67      0.80         3

    accuracy                           0.60         5
   macro avg       0.50      0.56      0.49         5
weighted avg       0.70      0.60      0.61         5

>>> y_pred = [1, 1, 0]
>>> y_true = [1, 1, 1]
>>> print(classification_report(y_true, y_pred, labels=[1, 2, 3]))
              precision    recall  f1-score   support

           1       1.00      0.67      0.80         3
           2       0.00      0.00      0.00         0
           3       0.00      0.00      0.00         0

   micro avg       1.00      0.67      0.80         3
   macro avg       0.33      0.22      0.27         3
weighted avg       1.00      0.67      0.80         3
```

https://scikit-learn.org/stable/modules/generated/sklearn.metrics.classification_report.html

F1 SCORE

- To fully evaluate the effectiveness of a model, you must examine **both** precision and recall

- F1 score is the harmonic mean of precision and recall

$$F_1 = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}} = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} = \frac{TP}{TP + \frac{FN + FP}{2}}$$

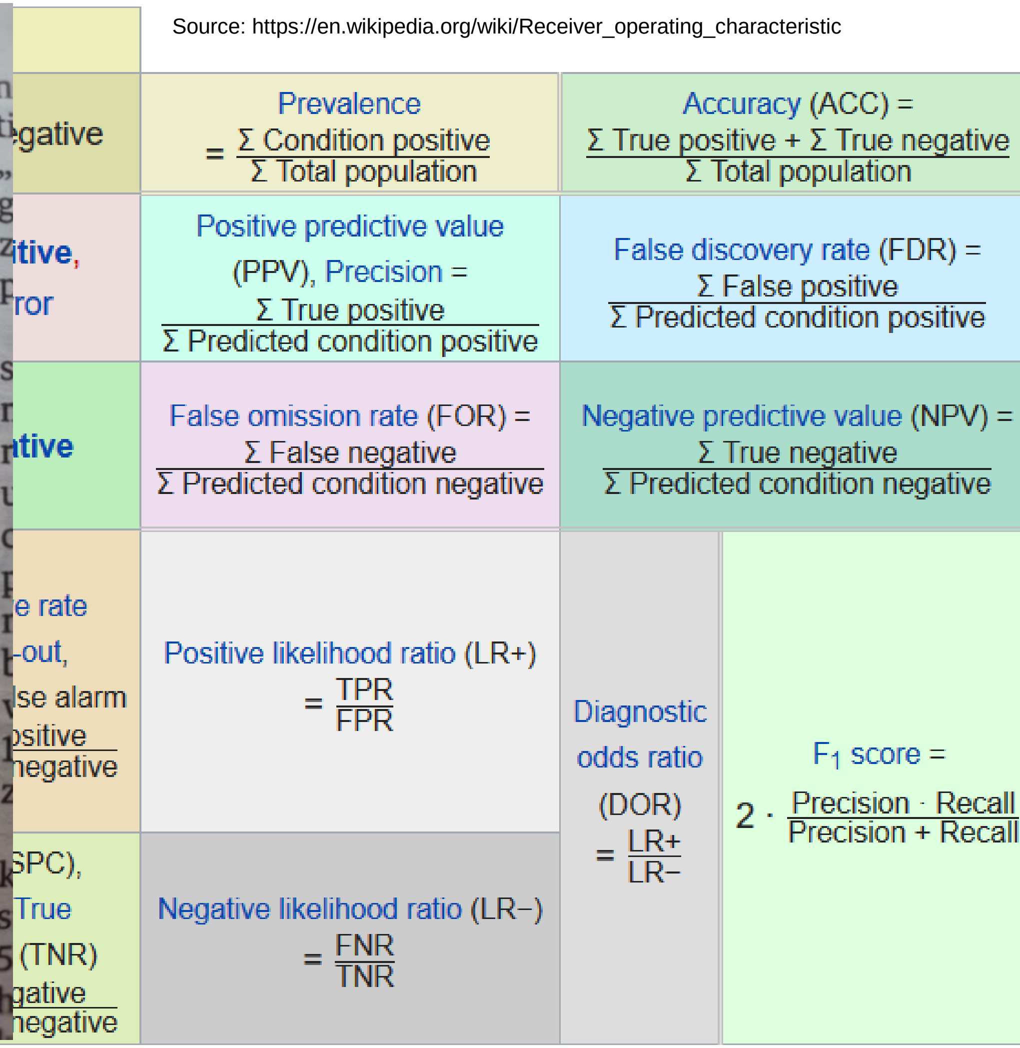
MANY METRICS

veren. Alle tests van de deelnemende partijen zijn eerst beoordeeld door het RIVM. „We sturen tien monsters, vijf met SARS-CoV-2 in verschillende concentraties, drie met andere coronavirussen, en twee waar niets in zit. De labs weten niet wat waar in zit. Als hun uitslagen kloppen, is de test goed”, zegt Reusken.

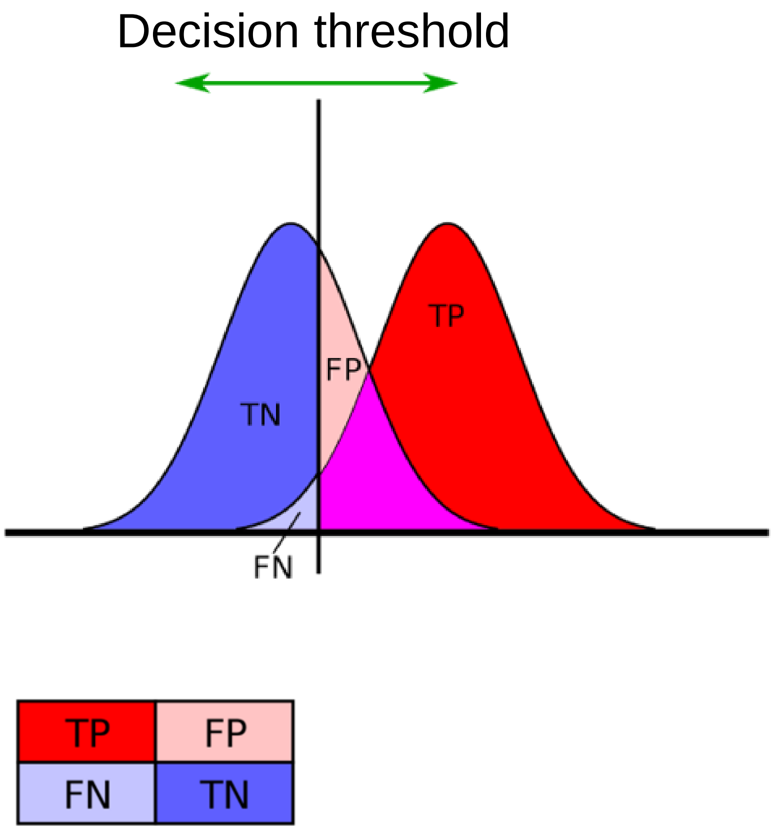
De testprestaties zullen per lab wat variëren: de specificiteit (de kans dat je een niet-ziek iemand ook als niet-ziek detecteert) en de sensitiviteit (de kans dat je een ziek iemand als ziek detecteert). De E-gen test is gevoeliger dan de RdRP-gen test, maar wat minder specifiek: naar schatting 99 tot 99,5 procent. Tests op meerdere genen zijn iets specifieker. Door de variatie ligt die specificiteit landelijk minimaal op 99,5 procent, zegt Reusken.

4 | Wat bepaalt hoeveel foute uitslagen een test geeft?

„De specificiteit hangt af van de test zelf



PRECISION/RECALL TRADE-OFF



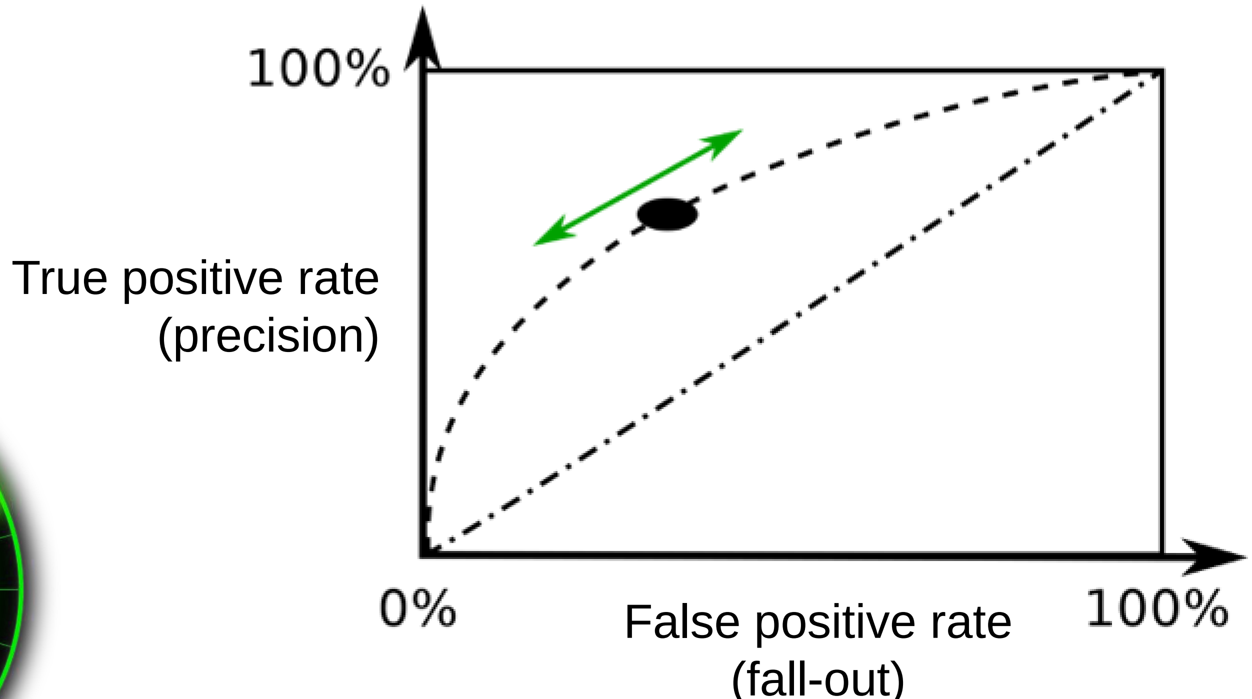
$$\text{precision} = \frac{TP}{TP + FP} \qquad \text{recall} = \frac{TP}{TP + FN}$$

Source: https://en.wikipedia.org/wiki/Tug_of_war#/media/File:Touwtrekken.jpg

Source: https://en.wikipedia.org/wiki/Receiver_operating_characteristic#/media/File:ROC_curves.svg

ROC CURVE

- *probability of detection* vs *probability of false alarm* at different decision thresholds.



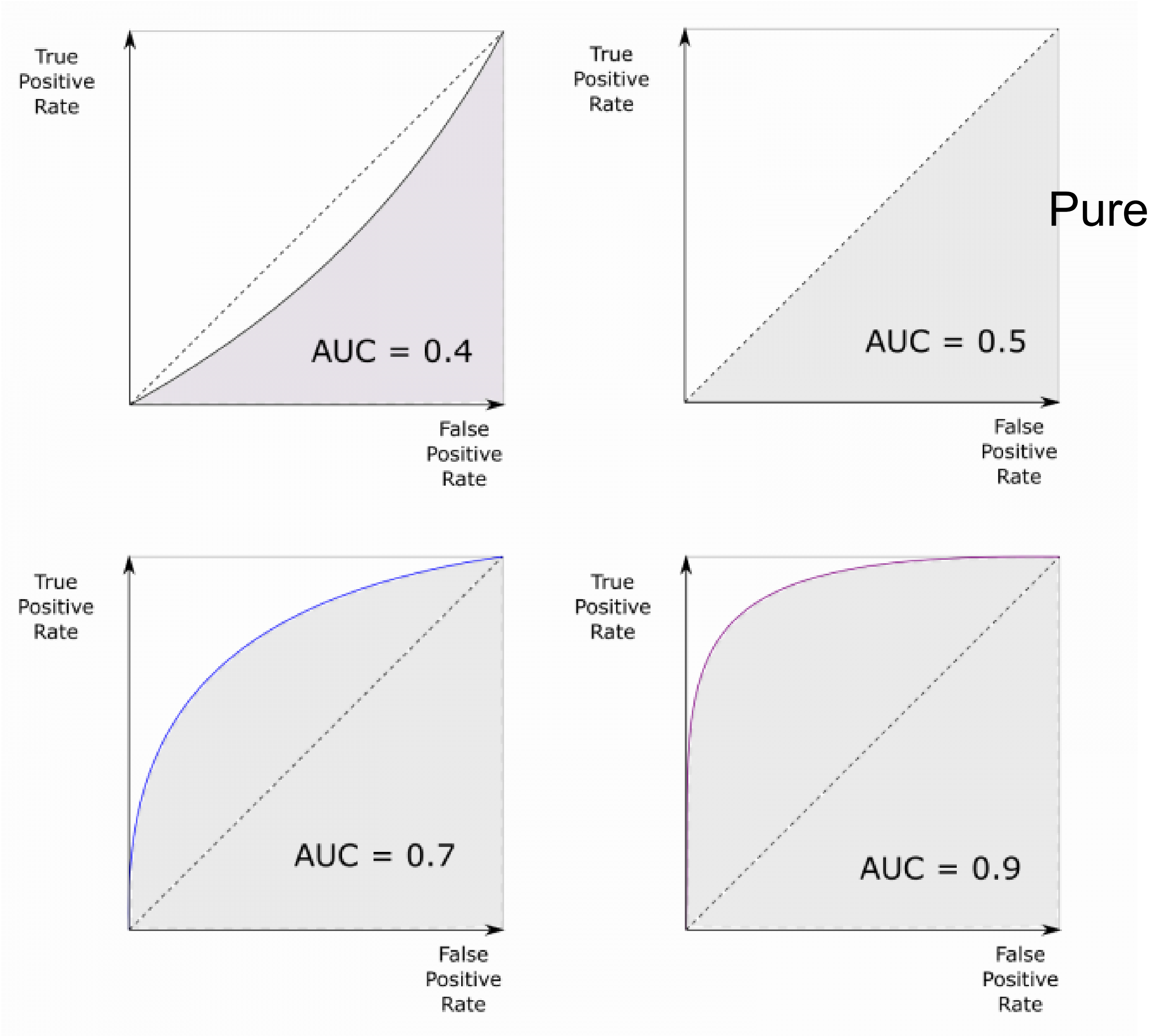
Source: https://en.wikipedia.org/wiki/Receiver_operating_characteristic#/media/File:ROC_curves.svg

COST OF CLASSIFICATION

- Sometimes false negatives don’t hurt as much as false positives Think of a poisonous mushroom detector….

- Use the ROC curve (receiver operating characteristics) to help balance the cost of classification

ROC AREA UNDER THE CURVE (AUC)



Purely random…

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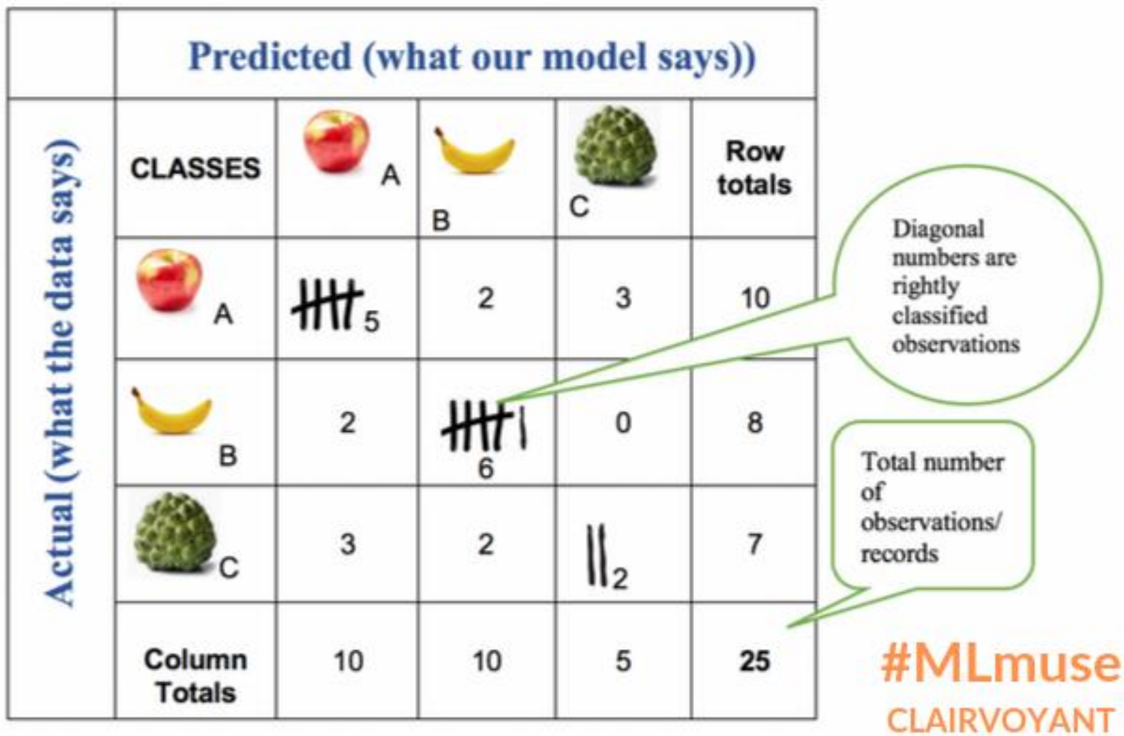
MULTICLASS CONFUSION MATRIX



Actual (what the data says)	Predicted (what our model says))				
	CLASSES	A	B	C	Row totals
	A	5	2	3	10
	B	2	6	0	8
	C	3	2	2	7
	Column Totals	10	10	5	25

Source: https://miro.medium.com/max/1400/1*jtoE1zEJaG0JvGlX3jOTFQ.png

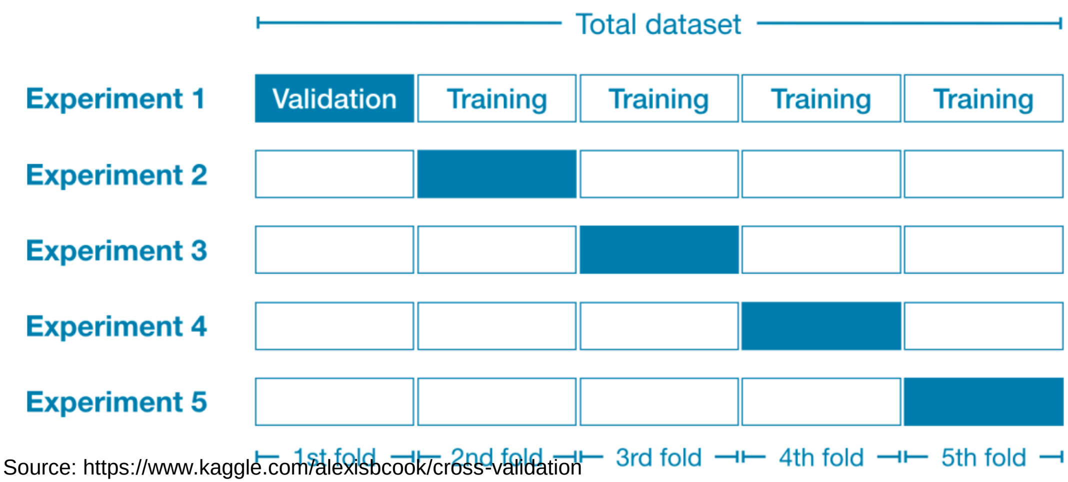
SPLITTING DATA

- Slice data into three subsets: Training, validation and test data

- Make sure that your subsets meet the following conditions:
  - Large enough to yield statistically meaningful results.
  - Representative of the data set as a whole.
    E.g. don't pick a test set with different characteristics than the training set.

CROSS-VALIDATION

- Estimate of a model’s generalization performance
- Break the data into folds

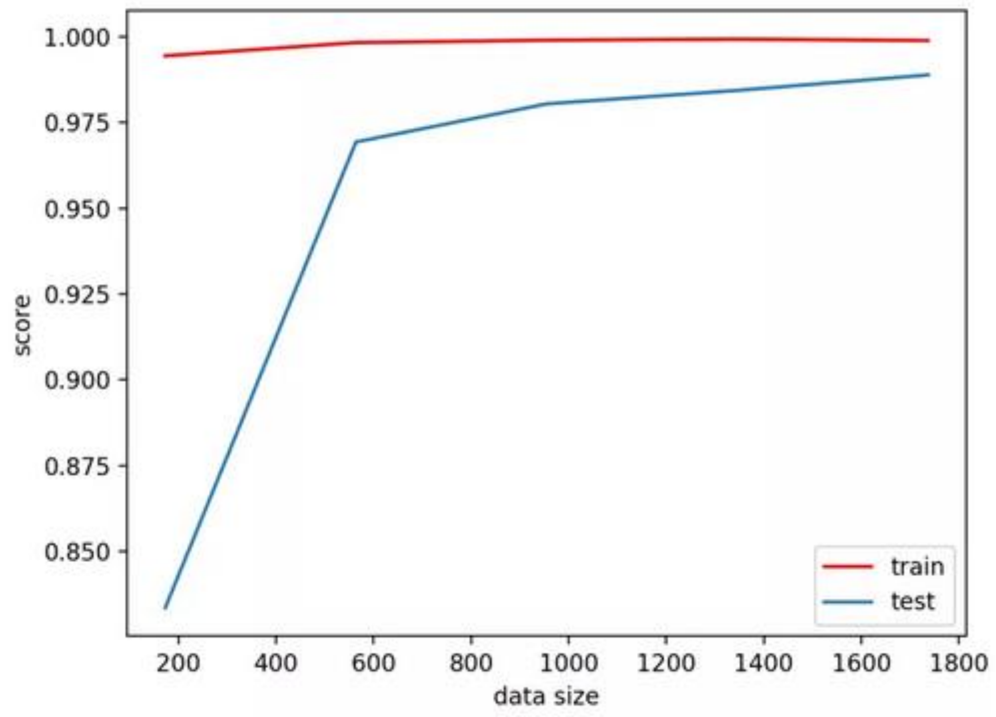


Source: https://www.kaggle.com/alexisbcook/cross-validation

- For small datasets, where extra computational burden isn't a big deal, you should run cross-validation.

LEARNING CURVES

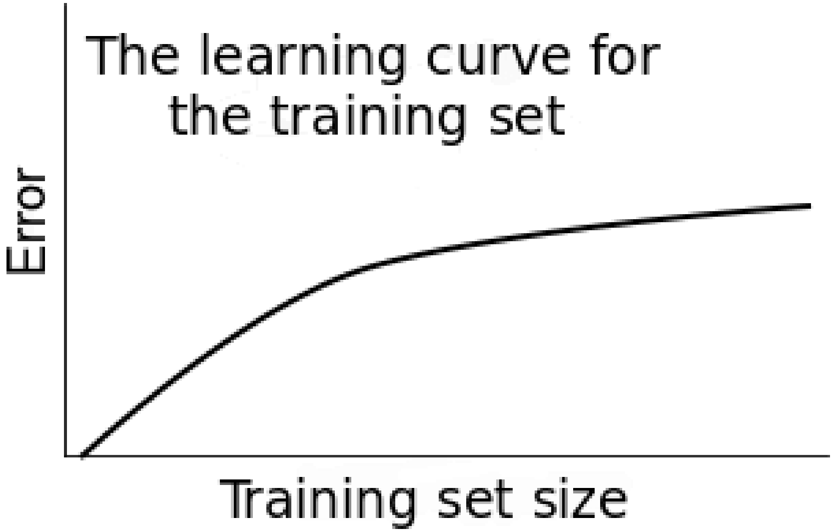
- A powerful diagnostic tool!

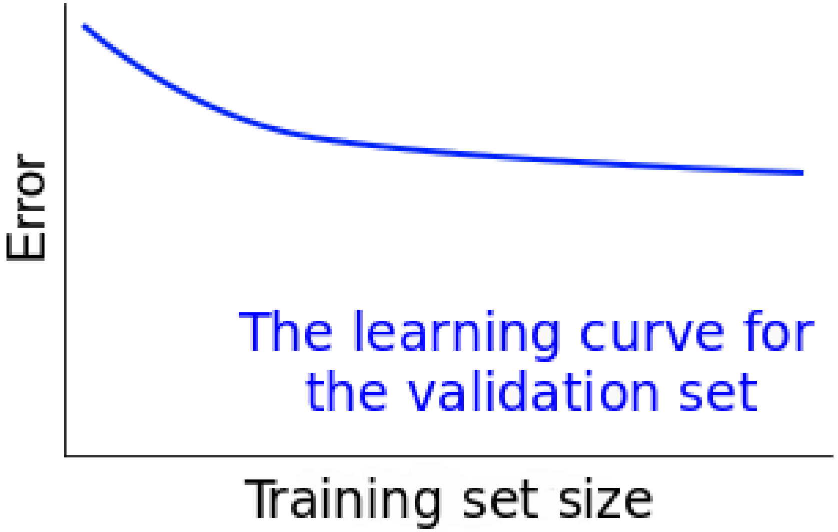



```
from sklearn.model_selection import learning_c
from sklearn.svm import SVC
from sklearn.datasets import load_digits
from matplotlib import pyplot as plt
import numpy as np

X, y = load_digits(return_X_y=True)
estimator = SVC(gamma=0.001)

train_sizes, train_scores, test_scores, fit_times, _ = learning_curve(estimator, X, y, cv=30,return_times=True)

plt.plot(train_sizes,np.mean(train_scores,axis=1))
```

LEARNING CURVES

- Cost as a function of the training set size (or the training iteration)
- Examine evolution of train and validation learning curves

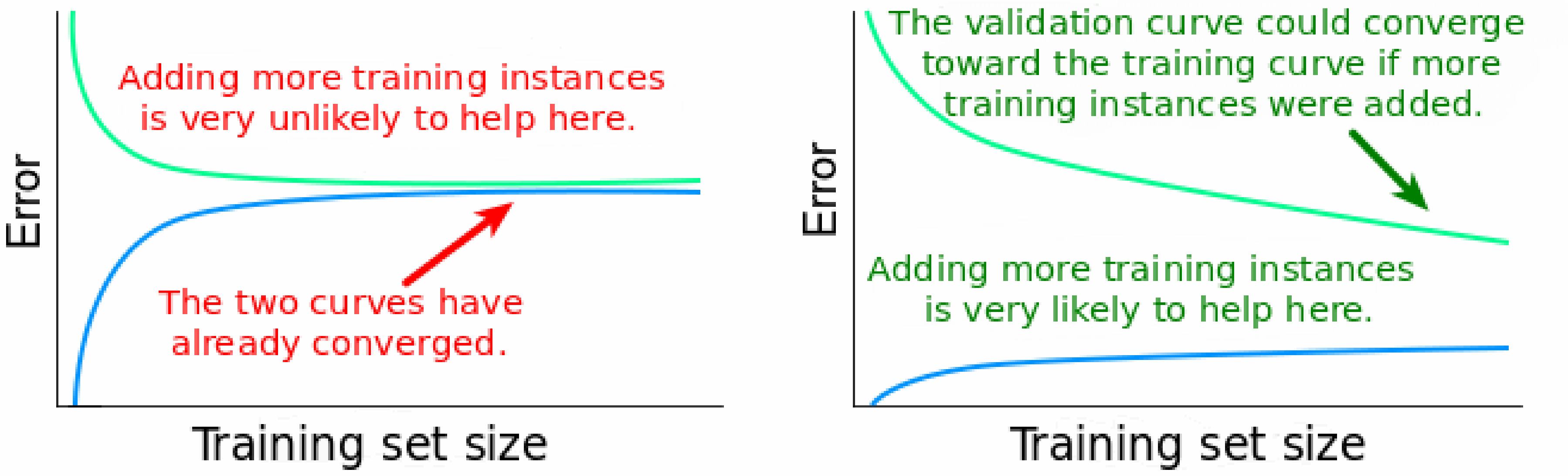




Source: https://www.dataquest.io/blog/learning-curves-machine-learning/

LEARNING CURVES

- Convergence of curves



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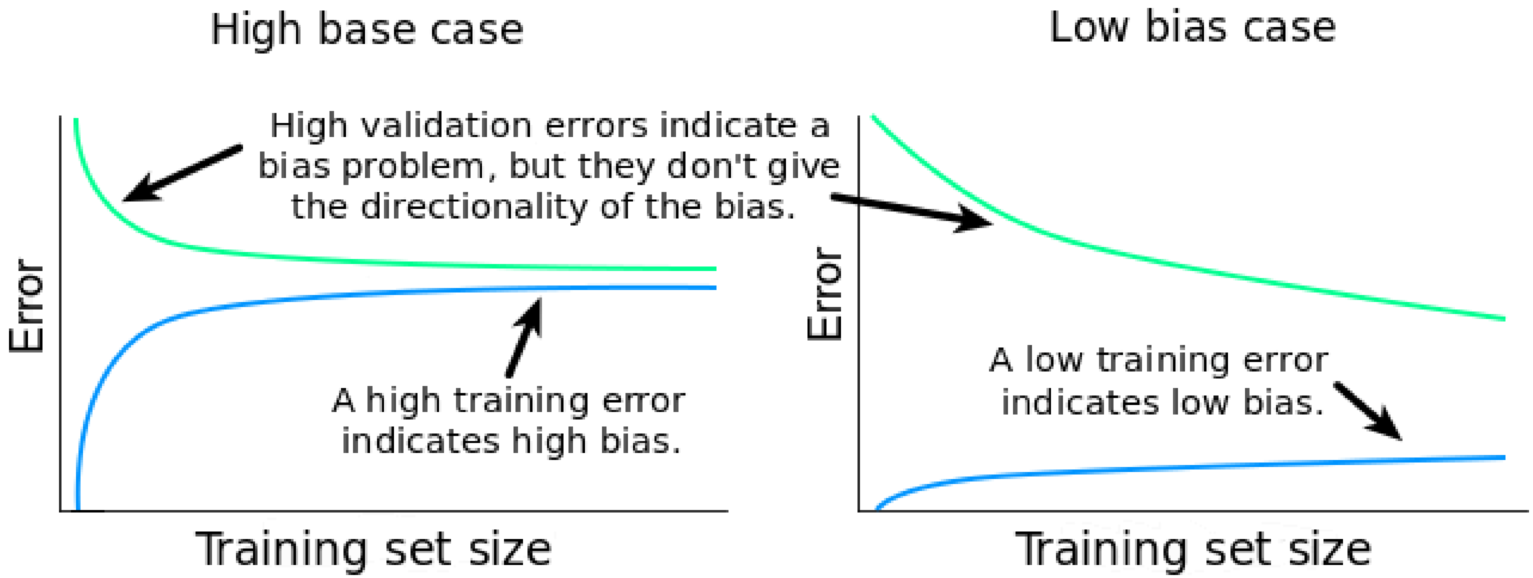
BIAS PROBLEM

- High validation error indicates a prediction bias problem
- Underfitting usually gives high bias



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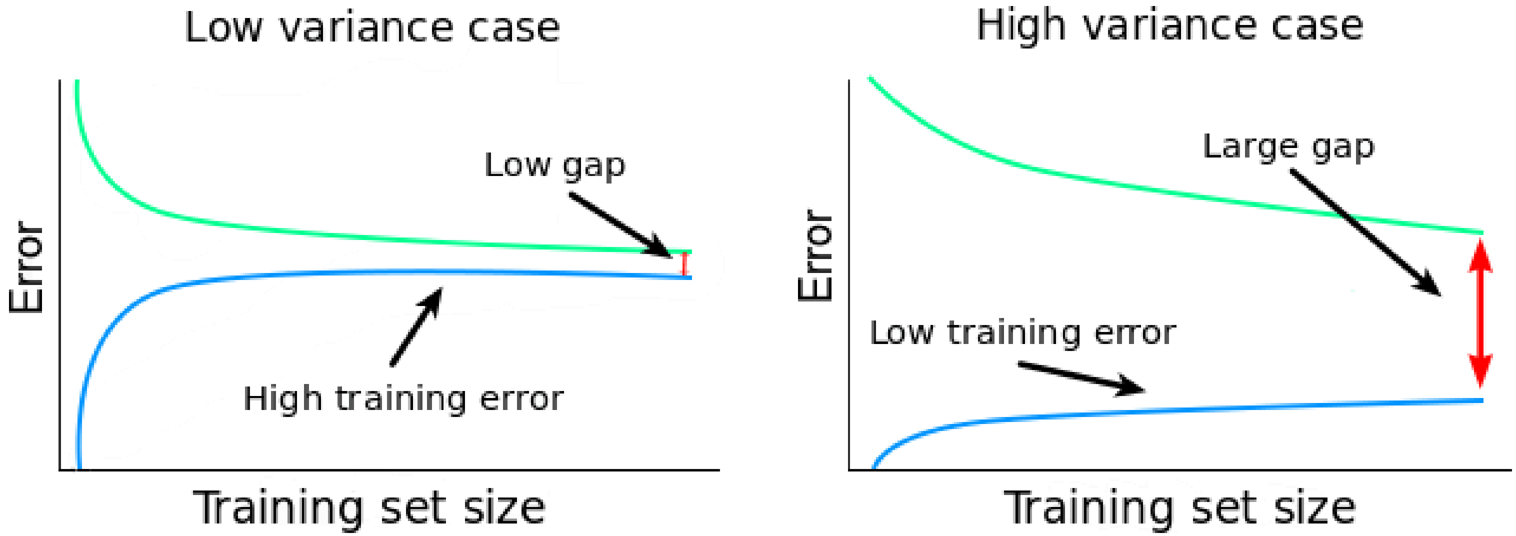
VARIANCE PROBLEM

- Low gap indicates low prediction variance
- Overfitting usually gives high variance



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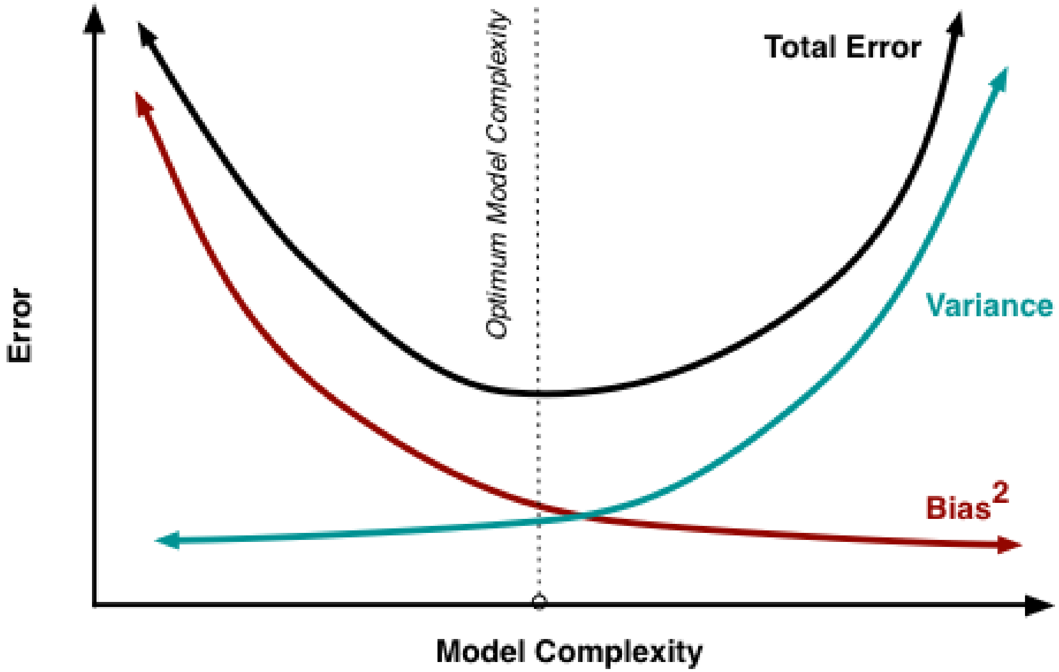
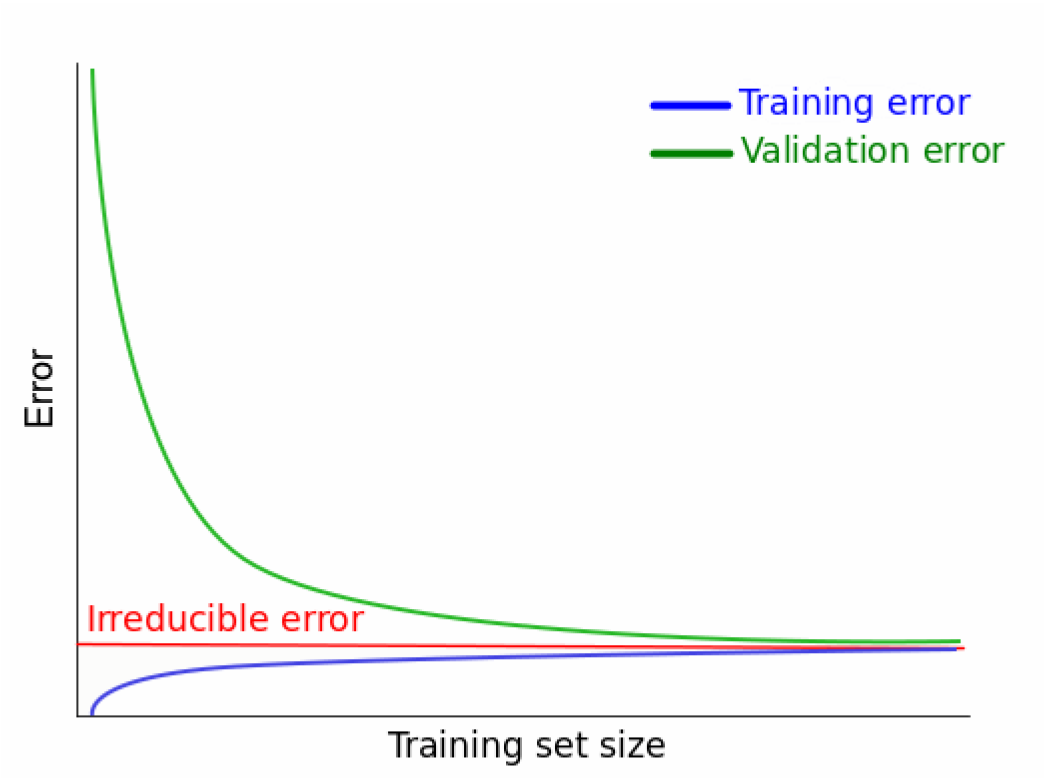
PREDICTION BIAS–VARIANCE TRADEOFF

- Central problem in supervised learning



IRREDUCIBLE ERROR

- Noise
- Cannot be predicted
- Loss cannot be reduced
- Outliers



Source: https://www.dataquest.io/blog/learning-curves-machine-learning/

MORE ON PREDICTION BIAS

- Average of predictions ≈ average of labels in test set

- A significant difference shows there is bias

- Possible causes:
  - Underfitting, e.g. incomplete feature set, overly strong regularization
  - Biased training samples
  - (Noisy data set)

QUESTION

- We know that on average, 1% of all emails are spam.
- My spam filter predicts that 20% of my incoming mail is spam.

What can we say about my spam filter?

COMPUTING CROSS-VALIDATED METRICS

- Predefined scoring parameters

Scoring	Function	Comment
Classification		
'accuracy'	`metrics.accuracy_score`	
'balanced_accuracy'	`metrics.balanced_accuracy_score`	
'average_precision'	`metrics.average_precision_score`	
'neg_brier_score'	`metrics.brier_score_loss`	
'f1'	`metrics.f1_score`	for binary targets
'f1_micro'	`metrics.f1_score`	micro-averaged
'f1_macro'	`metrics.f1_score`	macro-averaged
'f1_weighted'	`metrics.f1_score`	weighted average
'f1_samples'	`metrics.f1_score`	by multilabel sample
'neg_log_loss'	`metrics.log_loss`	requires `predict_proba` support
'precision' etc.	`metrics.precision_score`	suffixes apply as with 'f1'
'recall' etc.	`metrics.recall_score`	suffixes apply as with 'f1'
'jaccard' etc.	`metrics.jaccard_score`	suffixes apply as with 'f1'
'roc_auc'	`metrics.roc_auc_score`	
'roc_auc_ovr'	`metrics.roc_auc_score`	

See: https://scikit-learn.org/stable/modules/model_evaluation.html