Rensselaer

why not change the world?®

# Generalization, Overfitting, Model Validation

Ahmed Eleish

## Data Analytics ITWS-4600/ITWS-6600/MATP-4450/CSCI-4960

## October 10th 2024

Tetherless World Constellation
Rensselaer Polytechnic Institute

# Errors in Classification

- We've seen classification errors working with the iris/abalone classification examples
- Now we will take a look at what are the possible errors that take place in classification.
- **If the predicted class label is different from the actual class label (true class) then there is an error with that classification**.
- In classification, the model's output is the predicted class label for the input variables and the true class label is the target.

# Misclassification Error

- The error rate is the percentage of errors made over the entire dataset
- Error rate is also known as the misclassification rate or simply called the error.
- Error = $(Number\ of\ Errors)/(Total\ Number\ of\ Samples)$

# Training, test and validation sets

- Training: subset of dataset used as input to the model's training algorithm
- Validation: subset used to evaluate models during training
- Test: subset used to test the final model

e.g. the training set (70%) is used to train multiple models (different features, parameters, etc.) and the validation set (20%) is used to compare and select the best performing model. The test set (10%) is then used to evaluate the selected model.

# Terminology Confusion!

- ‘Test’ and ‘validation’ are used interchangeably in academia and industry!
- That’s fine… make sure to know the proper use.
- In this class:
  - While training the dataset is split into 2 subsets: training & test.
  - A validation set may be kept out of the training process for final evaluation, but this is not required for your labs/assignments.

https://en.wikipedia.org/wiki/Training,_validation,_and_test_data_sets

# Errors

- The error on the training data is called as the “**training error**”
- The error on the test data is referred to as the **”test error”**
- **The error on the test data is a good indication of how well the classifier will perform on new data and this is known as the generalization**.
- If the classifier performs well on the new data, then it is a good generalization. Generalization refers to how well the model is performing on the new data (**data not used to train the model**)

# Test error : Generalization error

- If the model generalizes well, then it will perform well on the new data sets that has the *similar structure* to the training data..

- Since the Test error is an indication of how well the model generalizes to new data, *the test error also called the generalization error.*

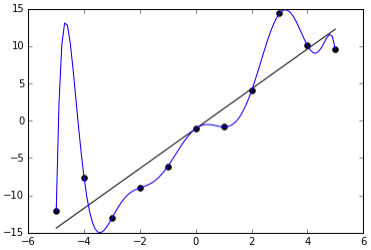
# Overfitting

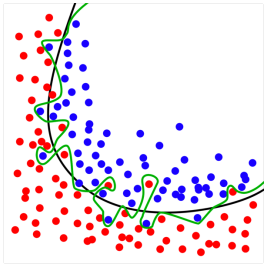
- Another related concept to Generalization is “overfitting”.
- If the model has very low training error but it has high generalization error, then it is over fitting.


Resource/Reference: Introduction to Statistical Learning with R, 7th Edition

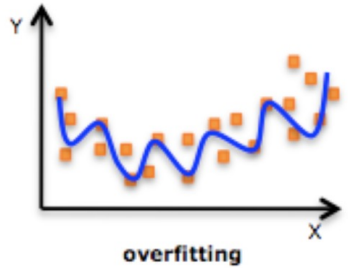
# Overfitting

- This is a good indication that the model may have learned to ***model the noise*** in the training data, instead of the learning from the underlying structure of the data.
- Overfitting is an indication of poor generalization.

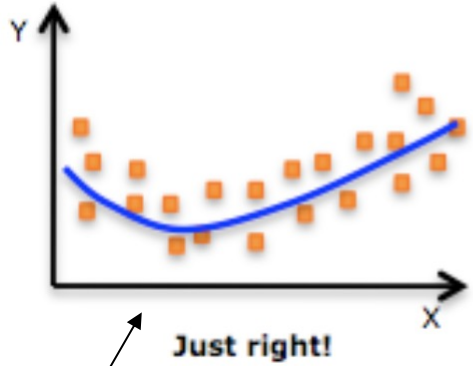


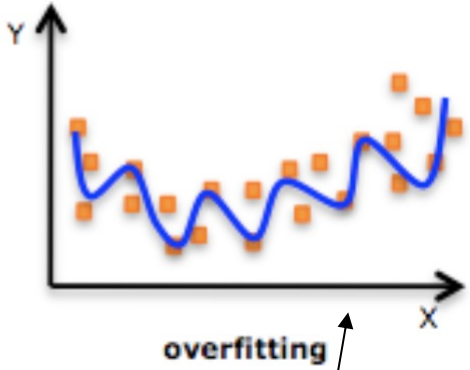
Image/Photo Credit:
https://en.wikipedia.org/wiki/Overfitting#/media/File:Overfitted_Data.png




Image/Photo Credit:
http://pingax.com/regularization-implementation-r/




Model is fitting to
the structure of the data



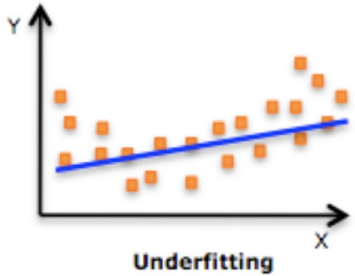

Model is fitting to
the noise of the data



Image/Photo Credit: http://pingax.com/regularization-implementation-r/

# Underfitting

- **Underfitting** occurs when a statistical model cannot adequately capture the underlying structure of the data.
- In other words, **underfitting take place when the model has not properly learned the structure of the data**.




Image/Photo Credit: http://pingax.com/regularization-implementation-r/

# Robustly Validating Models

- There are several ways to create the evaluate/validate models
  - Holdout method
  - K-fold Cross validation
  - Monte Carlo Cross validation
  - Leave-One-Out Cross validation

# Holdout Method

- Split the dataset into 2 subsets, one for training and another for testing.
- The training set is usually larger than the test set.
- Not recommended for robust validation.

# K-fold Cross Validation

- In k-fold cross validation, the data are segmented in to *k* number of **disjoint partitions**.
- During each iteration, one partition is used as the test set and the remaining k-1 (combined) for training; The process is repeated *k* times.
- Each time using a different partition for testing, so that each partition is used exactly one time for the validation.


Resource/Reference: Introduction to Statistical Learning with R, 7th Edition - Chapter 5

# Monte Carlo Cross Validation (Repeated random sub-sampling)

- In Monte Carlo cross validation, the dataset is split into training/test sets over *n* iterations with the samples in each selected at random.
- The size of each partitions may be constant or vary over the iterations.
- Commonly used in research, considered robust because of the averaging effect over multiple iterations.
- Downside: since selection is random, some observations may not end up in test sets and some may be oversampled

Resource/Reference: Introduction to Statistical Learning with R, 7th Edition - Chapter 5

# Leave One Out Cross Validation (LOOCV)

- For as many iterations as there are observations, drop one observation and used all the others for training; test one the 1 observation and average at the end.

- Depending on the size of the dataset, may be computationally expensive.

Resource/Reference: Introduction to Statistical Learning with R, 7th Edition - Chapter 5

# Thanks!
# Have a great weekend!

Work on your assignment/project proposal!!!