K NEAREST NEIGHBORS

BEFORE WE BEGIN: LET US RUN AN EXPERIMENT

I need two volunteers who are willing to reveal their political opinion and for which party they would vote, if we had elections today (ideally one Democrat and one Republican).

The survey questions are below (wait for instructions before you take the survey and record your answers from the digital survey also on a piece of paper):

- Survey for all students (except the two volunteers): https://tinyurl.com/KNearNeighTrain
- Survey for the two volunteers https://tinyurl.com/KNearNeighTest

IDEAS ON HOW TO IDENTIFY THE 2 VOLUNTEERS POLITICAL AFFILIATION?

- CL: Ask volunteers what their answers were and find nearest neighbor(s) (volunteers: do not reveal political affiliation yet).
- What were the shortcomings of the survey
- CL: Run R Script

OVERWIEW

In this session you will learn:

- 1. What is the underlying idea of k-Nearest Neighbors
- 2. How similarity can be measured with **Euclidean distance**
- 3. Why scaling predictor variables is important for some machine learning models
- 4. Why the **tidymodels package** makes it easy to work with machine learning models
- 5. How you can define a **recipe** to pre-process data with the tidymodels package
- 6. How you can define a **model-design** with the **tidymodels** package
- 7. How you can create a machine learning **workflow** with the tidymodels package
- 8. How **metrics** derived from a **confusion matrix** can be used to asses prediction quality
- 9. Why you have to be careful when interpreting *accuracy*, when you work with **unbalanced observations**
- O. How a machine learning model can **process images** and how OCR (Optical Character Recognition) works»

ABOUT THE WINE DATASET

We will work with a publicly available 'wine dataset¹ containing 3,198 observations about different wines and their chemical properties.

Our goal is to develop a k-Nearest Neighbors model that can predict if a wine is red or white based on the wine's chemical properties.»

RAW OBSERVATIONS FROM WINE DATASET

- 1 library(rio)
- 2 DataWine=import("https://ai.lange-analytics.com/data/WineData.rds")
- 3 print(DataWine)

	wineColor	acidity	volatileAcidity	citricAcid	residualSugar	Chlorides
1	red	10.80	0.320	0.44	1.60	0.063
2	white	6.40	0.310	0.39	7.50	0.040
3	white	9.40	0.280	0.30	1.60	0.045
4	white	8.20	0.220	0.36	6.80	0.034
5	white	6.40	0.290	0.44	3.60	0.197
6	red	6.70	0.855	0.02	1.90	0.064
7	red	11.80	0.380	0.55	2.10	0.071
8	white	6.70	0.250	0.23	7.20	0.038
9	red	7.50	0.380	0.57	2.30	0.106
10	red	7.10	0.270	0.60	2.10	0.074
11	white	6.40	0.270	0.19	1.90	0.085
12	red	7.80	0.600	0.26	2.00	0.080
13	red	8.00	0.580	0.28	3.20	0.066
14	white	7.00	0.360	0.35	2.50	0.048
15	red	9.90	0.440	0.46	2.20	0.091
16	white	7.80	0.280	0.31	2.10	0.046
17	rad	7 60	Λ ΔΛΛ	n 29	1 90	N N78



OBSERVATIONS FROM WINE DATASET FOR SELECTED VARIABLES SULFOR DIOXIDE AND ACIDITY

Note we use clean names ("upper_camel") from the janitor package to change all column (variable) names to UpperCamel.

```
1 library(tidyverse); library(rio); library(janitor)
  DataWine=import("https://ai.lange-analytics.com/data/WineData.rds") %>%
    clean names ("upper camel") %>%
3
    select (WineColor, Sulfur=TotalSulfurDioxide, Acidity) %>%
    mutate(WineColor=as.factor(WineColor))
  print(DataWine)
```

```
WineColor Sulfur Acidity
         red 37.0 10.80
       white 213.0
                  6.40
       white 139.0 9.40
       white 90.0 8.20
       white 183.0 6.40
         red 38.0
                   6.70
         red 19.0
                   11.80
       white 220.0
                  6.70
         red 12.0 7.50
         red 25.0
                    7.10
10
       white 196.0 6.40
12
         red 131.0
```

https://ai.lange-analytics.com/

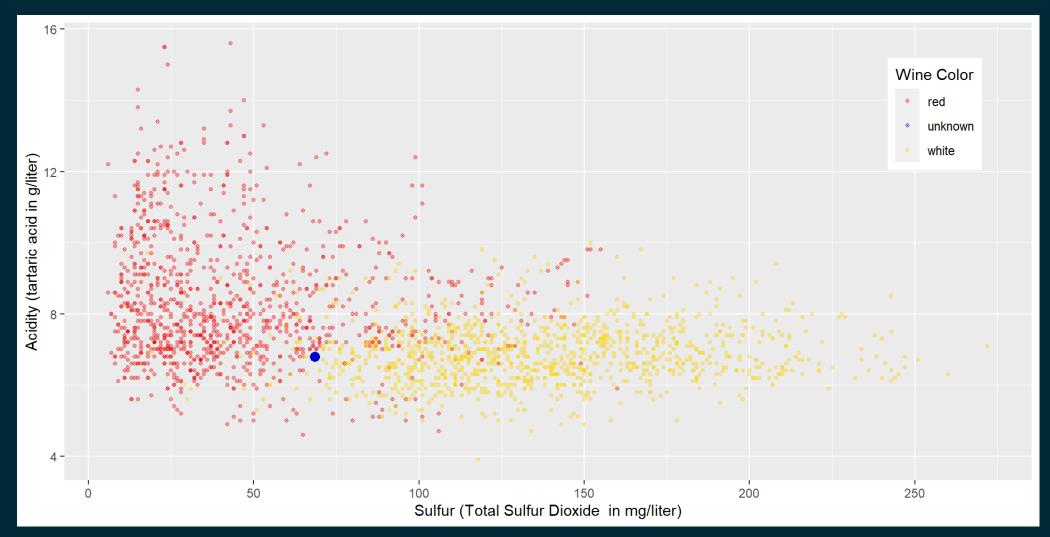
13	red	114.0	8.00
14	white	161.0	7.00
15	red	41.0	9.90
16	white	208.0	7.80

BEFORE STARTING WITH K NEAREST NEIGHBORS

LET US FIND SOME EYEBALLING TECHNIQUES THAT ARE RELATED TO VARIOUS MACHINE LEARNING MODELS»

EYE BALLING TECHNIQUES TO IDENTIFY RED AND WHITE WINES

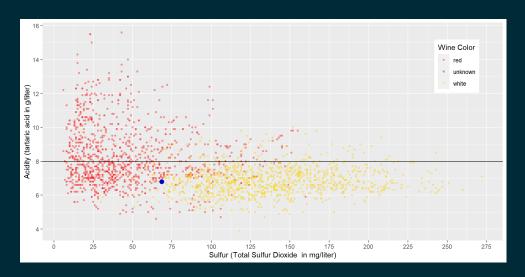
TRY EYEBALLING THE TRAINING DATA (N=2238)



Acidity and Total Sulfur Dioxide Related to Wine Color

EYE BALLING TECHNIQUES TO IDENTIFY RED AND WHITE WINES

HORIZONTAL BOUNDARY



Horizontal Decision Boundary for Acidity and Total Sulfur Dioxide Related to Wine Color

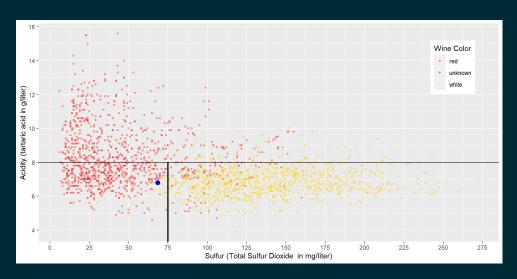
CONFUSION MATRIX

```
Truth
Prediction red white
red 510 80
white 609 1039
```

ACCURACY

EYEBALLING TECHNIQUES TO IDENTIFY RED AND WHITE WINES

CREATING SUBSPACES LIKE SIMILAR TO A DECISION TREE



Sub-Space Boundaries for Acidity and Total Sulfur Dioxide Related to Wine Color

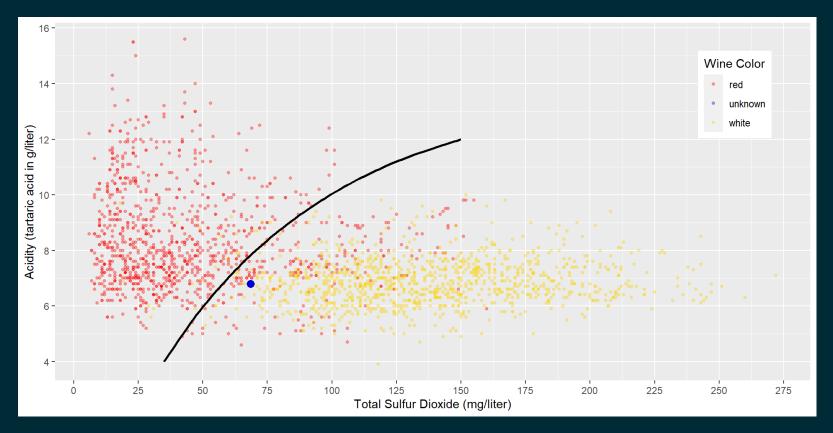
CONFUSION MATRIX

```
Truth
Prediction red white
red 1016 145
white 103 974
```

ACCURACY

EYEBALLING TECHNIQUES TO IDENTIFY RED AND WHITE WINES

USING A NON-LINEAR DECISION BOUNDARY LIKE A NEURAL NETWORK



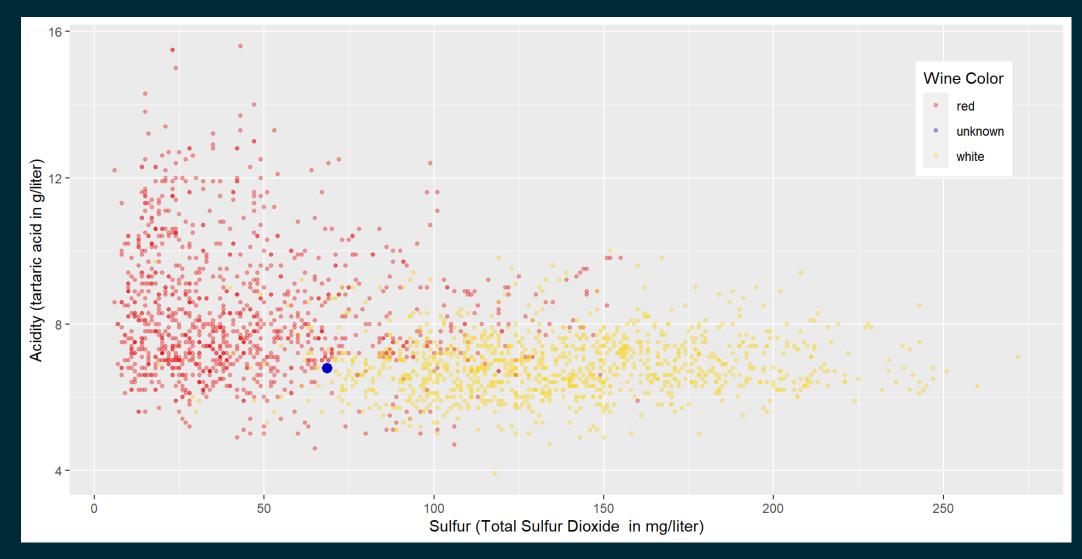
Curved Decision Boundary for Acidity and Total Sulfur Dioxide Related to Wine Color

CONFUSION MATRIX AND ACCURACY

Similar as previous one.

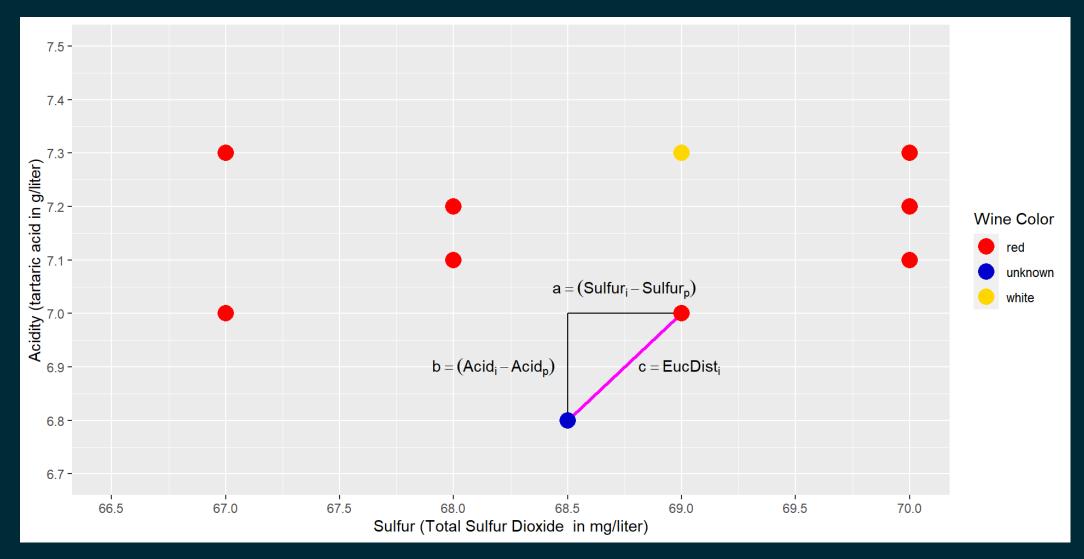
SO, HOW DOES K NEAREST NEIGHBORS WORK?

K NEAREST NEIGHBORS K=1



Acidity and Total Sulfur Dioxide Related to Wine Color»

K NEAREST NEIGHBORS K=1



Predicting Wine Color with k-Nearest Neighbors (k=1)

HOW TO CALCULATE EUCLIDEAN DISTANCE FOR TWO VARIABLES

Assume our observations have **two predictor variables** x and y. We compare the unknown point p to one of the points from the training data (e,g., point i):

$$Dist_i = \sqrt{(x_p-x_i)^2+(y_p-y_i)^2}$$

>>

HOW TO CALCULATE EUCLIDEAN DISTANCE FOR THREE VARIABLES

Assume our observations have **three predictor variables** x, y, and z. We compare the unknown point p to one of the points from the training data (e,g., point i):

$$Dist_i = \sqrt{(x_p - x_i)^2 + (y_p - y_i)^2 + (z_p - z_i)^2}$$

>>

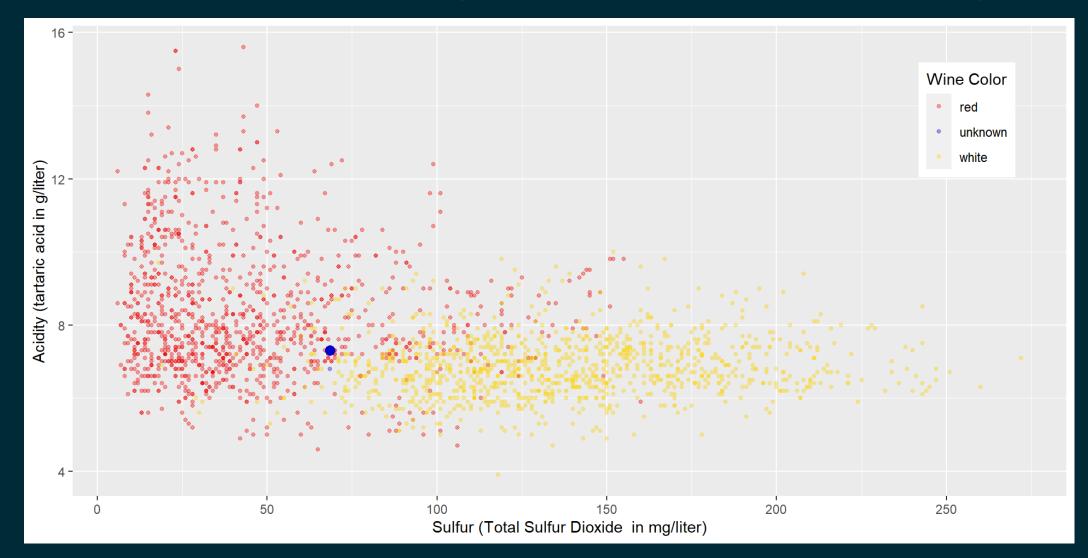
HOW TO CALCULATE EUCLIDEAN DISTANCE FOR N VARIABLES

Assume our observations have N predictor variables v_j with j=1...N. We compare the unknown point p to one of the points from the training data (e,g., point i):

$$Dist_i = \sqrt{\sum_{j=1}^N (v_{p,j} - v_{i,j})^2}$$

>>

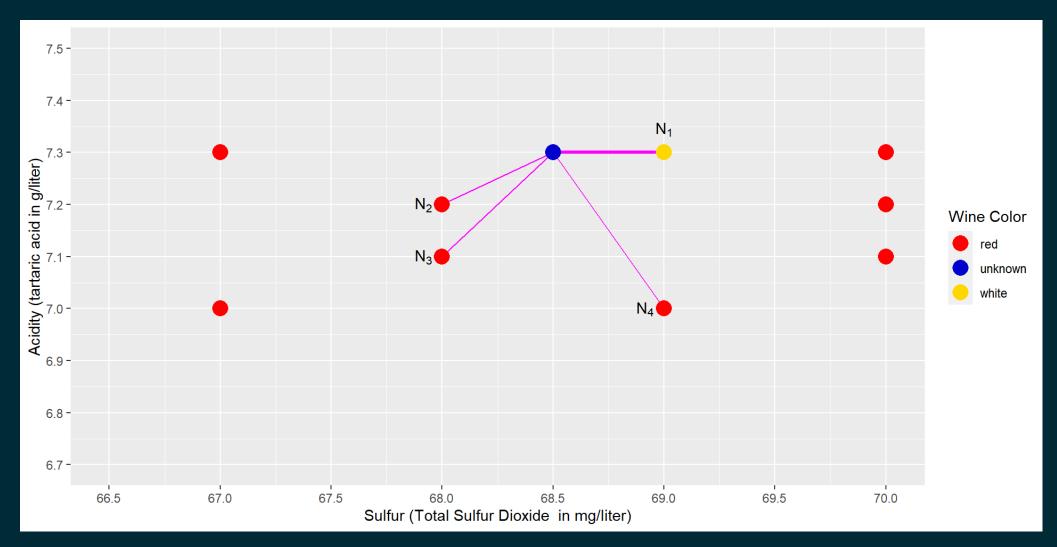
K NEAREST NEIGHBORS K=4 (FOR A DIFFERENT UNKNOWN WINE)



Acidity and Total Sulfur Dioxide Related to Wine Color

K NEAREST NEIGHBORS K=4 (FOR A DIFFERENT UNKNOWN WINE)

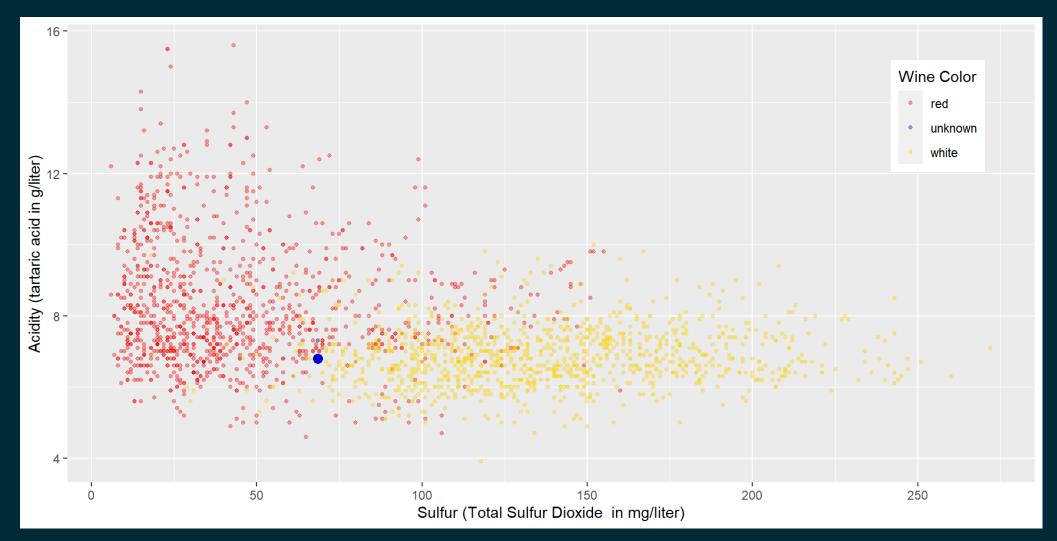
4 NEAREST NEIGHBORS VOTE ON "RED" VS. "WHITE"



Predicting Wine Color with k-Nearest Neighbors (k=4)

K NEAREST NEIGHBORS K=4 (FOR A DIFFERENT UNKNOWN WINE)

WATCH THE SCALE: G/LITER VS. MG/LITER. THAT DOES NOT LOOK RIGHT!



Acidity and Total Sulfur Dioxide Related to Wine Color »

A FEW COMMON SCALING OPTIONS

Convert from sub-units to major units or vice versa by multiplying or deviding

For example, if one variable is in feet and one in inches, you can multiply feet by 12 to get inches or devide inches by 12 to get feet. This is often not possible (e.g., Height and Weight).

Rescaling (R command range())

Generates a variable y that is scaled to a range between 0 and 1 based on the original variable's value x, its minimum x_{min} and its maximum x_{max} :

$$y=rac{x-x_{min}}{x_{max}-x_{min}}$$

Z-Score Normalization

Z-score normalization uses the mean (\overline{x}) and the standard deviation (s) of a variable to scale the variable x to the variable z:

$$z=rac{x-\overline{x}}{s}$$

LOADING DATA AND SELECTING VARIABLES

```
WineColor Sulfur Acidity
         red 37.0
                   10.80
       white 213.0 6.40
       white 139.0 9.40
                   8.20
       white 90.0
       white 183.0 6.40
         red 38.0 6.70
         red 19.0 11.80
       white 220.0
                   6.70
         red 12.0 7.50
         red 25.0
                     7.10
10
11
       white 196.0
                    6.40
         red 131.0
         red 114.0
14
       white 161.0
                     7.00
15
         red 41.0
                    9.90
16
       white 208.0
         red
```

Generate Training and Testing Data (Splitting):

```
1 library(tidymodels);
2 set.seed(876)
3 Split7030=initial_split(DataWine,prop=0.7,strata = WineColor)
4
5 DataTrain=training(Split7030)
6 DataTest=testing(Split7030)
7 print(DataTrain)
```

```
WineColor Sulfur Acidity
          red
               37.0
                      10.80
               38.0
                      6.70
          red
                      7.50
          red 12.0
          red 25.0
                      7.10
                      8.00
          red 114.0
          red 66.0
                    7.60
          red 49.0 6.80
          red 110.0
                      7.00
          red 44.0
                       6.50
10
          red
               10.0
                      10.40
          red 149.0
                      6.60
11
12
          red
              31.0
                      6.60
               49.0
                      6.60
13
          red
                     9.10
14
          red
               17.0
15
          red
               32.0 6.10
16
               30.0
                       8.50
          red
                                https://ai.lange-analytics.com/
          rad
```

1 print(DataTest)

	WineColor	Sulfur	Acidity
1	white	90.0	8.20
2	red	19.0	11.80
3	white	220.0	6.70
4	red	131.0	7.80
5	white	161.0	7.00
6	red	41.0	9.90
7	white	156.0	7.80
8	white	150.0	6.50
9	red	102.0	7.90
10	red	11.0	5.80
11	white	64.0	5.90
12	white	178.0	6.90
13	red	41.0	12.60
14	red	19.0	12.70
15	white	206.0	6.20
16	white	149.0	6.90
17	white	182 0	7 80

CLICK HERE TO FIND A REFERENCE LIST FOR VARIOUS Step_ COMMANDS

Recipe: Prepare Data for Analysis:

CLICK HERE TO FIND A REFERENCE LIST FOR VARIOUS Step_ COMMANDS

Creating a Model Design:

Putting it all together in a **fitted** workflow:

```
WFModelWine=workflow() %>%
                 add recipe(RecipeWine) %>%
                 add model (ModelDesignKNN) %>%
                 fit(DataTrain)
  5 print(WFModelWine)
Workflow [trained] =
Preprocessor: Recipe
Model: nearest neighbor()
- Preprocessor -
2 Recipe Steps
• step naomit()
• step normalize()
-- Model ---
Call:
kknn::train.kknn(formula = ..y \sim ., data = data, ks = min rows(4, data, 5), kernel =
~"rectangular")
Type of response variable: nominal
Minimal misclassification: 0 1000894
```

How to use the **fitted** workflow to predict the wine color for the wines in the testing dataset:

- 1. Start with observation i=1 from DataTest (the first observation).
- 2. Take observation i from DataTest and use Acidity and Sulfur to calculate the Euclidean distance to **each** of the observations of DataTrain.
- 3. Isolate the 4 observations with the smallest Euclidean distance and use the majority of their wine color as a prediction for observation i from DataTest (in case of a par, decide randomly).
- 4. Increase i by one (i.e., take the next observation from DataTest) and go to step 2 (until all DataTest observations are processed).

Predicting with the fitted workflow using predict() (not exactly helpful!):

```
1 predict(WFModelWine, DataTest)

# A tibble: 960 × 1
    .pred_class
    <fct>
1 white
2 red
3 white
4 white
5 white
6 red
7 white
8 white
9 red
10 red
# i 950 more rows
```

Predicting with the fitted workflow using augment() which augments DataTest with the predictions:

- 1 DataPredWithTestData=augment(WFModelWine, DataTest)
- 2 head (DataPredWithTestData)

```
\# A tibble: 6 \times 6
 WineColor Sulfur Acidity .pred class .pred red .pred white
 <fct>
          <dbl>
                <dbl> <fct>
                                  <dbl>
                                            <dbl>
1 white
                  8.2 white
            90
2 red
          19 11.8 red
3 white 220 6.7 white
                               0.25
4 red 131 7.8 white
        161 7
                     white
5 white
        41 9.9 red
6 red
```

HAVING A DATA FRAME WITH truth AND esimate WE CAN CALCULATE PERFORMANCE METRICS

Confusion Matrix:

1 ConfMatrixWine=conf_mat(DataPredWithTestData, truth = WineColor, estimate = .pred_clas
2 print(ConfMatrixWine)

```
Prediction red white red 436 46 white 44 434
```

READING THE CONFUSION MATRIX

```
Truth
Prediction Red Wine White Wine
Red Wine TP: 436 FP: 46
White Wine FN: 44 TN: 434
```

- The **positive class** (wine is "red") is in the **first column**. 436 of the positives are classified correctly (TR: true positives), and 44 positives are incorrectly classified (FN: false negatives).
- The **negative class** (wine is "white") is in the **second column**. 44 negatives are incorrectly classified (FP: false positives), and 434 negatives are classified correctly (TN: true negatives).

Accuracy: Number of wines on diagonal/number of all wines:

WARNING: BE CAREFUL WITH THE ACCURACY RATE

THE STORY OF DR. NEBULOUS'S GAMBLERS SYSTEM

Dr. Nebulous offers a **97% Machine Learning Gambling Prediction**. Here is how it works: Gamblers can buy a prediction for a fee of \$5. Dr. Nebulous will then run his famous machine learning model and send a closed envelope with the prediction. The gambler is supposed to open the envelope in the casino, right before placing a bet of \$100 on a number in roulette. The envelope contains a message that states either "You will win" or "You will lose", which allows the gambler to act accordingly by either bet or not bet.

Dr. Nebulous claims that a "clinical trial" of 1000 volunteers, who opened the envelope after they had bet on a number in roulette, shows an accuracy of 97.3%.

How could Dr. Nebulous have such a precise model?

WARNING: BE CAREFUL WITH THETHE ACCURACY RATE

THE STORY OF DR. NEBULOUS'S GAMBLERS SYSTEM

The trick is Dr. Nebulous's machine learning model uses the *naive* prognosis: It always predicts "You will lose".

Here is the confusion matrix from the 1,000 volunteers trial:

Roulette has 37 numbers to bet on. Chance to win is: $\frac{1}{37} = 0.027$.

Out of the 1000 volunteers, 27 are expected to win, and 973 are expected to lose.

$$Accuracy = \frac{0+973}{1000} = 0.973$$

WARNING: BE CAREFUL WITH THE ACCURACY RATE

THE STORY OF DR. NEBULOUS'S GAMBLERS SYSTEM

```
Truth
Prediction Win Lose
Win 0 0
Lose 27 997
```

However, when we look at the correct positive and the correct negative rate separately, we see that Dr. Nebulous' accuracy rate (although correct) makes little sense.

- The correct negative rate (**specificity**) is 100%
- The correct positive rate (**sensitivity**) is zero (out of the 27 winners, all were falsely predicted as "You will lose").

This example shows: When interpreting the confusion matrix, you must look at accuracy, sensitivity, and specificity simultaneously

accuracy(), sensitivity() and specificity() for the wine
data:

```
1 accuracy(DataPredWithTestData, truth = WineColor, estimate = .pred class)
\# A tibble: 1 \times 3
  .metric .estimator .estimate
 <chr> <chr>
                  <dbl>
1 accuracy binary 0.906
 1 sensitivity(DataPredWithTestData, truth = WineColor, estimate = .pred class)
# A tibble: 1 \times 3
  .metric .estimator .estimate
 <chr> <chr>
                          <dbl>
1 sensitivity binary
                           0.908
 1 specificity(DataPredWithTestData, truth = WineColor, estimate = .pred class)
# A tibble: 1 \times 3
  .metric .estimator .estimate
 <chr> <chr>
                           <dbl>
1 specificity binary 0.904
```

Can we improve by using all predictors.»

PROJECT: DESIGN A MACHINE LEARNING WORKFLOW FOR OPTICAL CHARACTER RECOGNITION >>

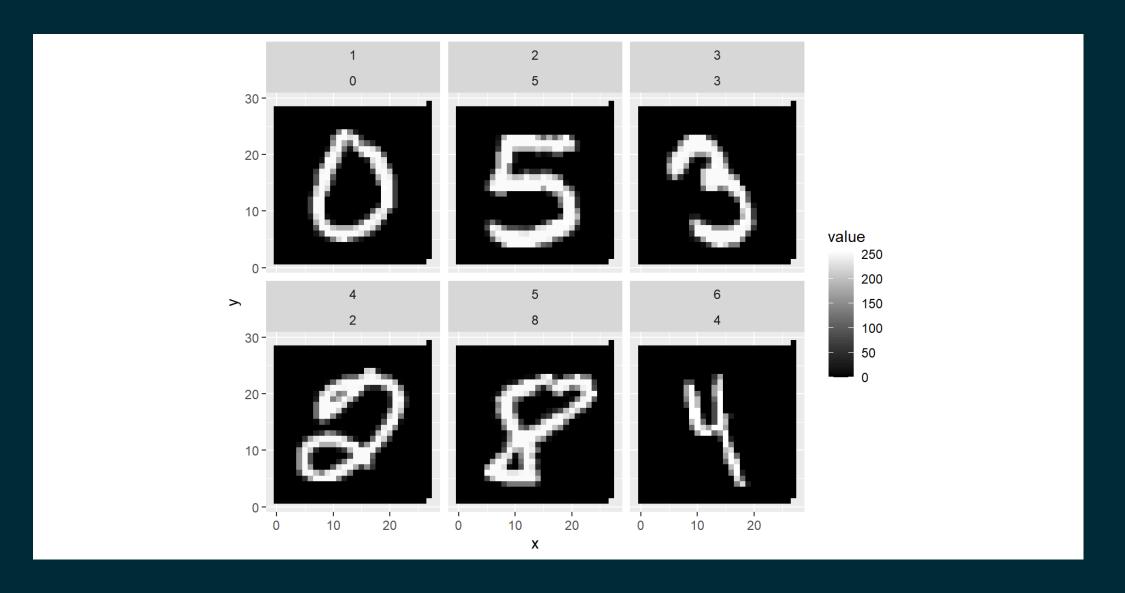
MNIST DATA SET

You will develop a machine learning model based on k-Nearest Neighbors to recognize handwritten digits from images.

You will use the MNIST dataset, a standard dataset for image recognition in machine learning (60,000 images for training and 10,000 images for testing). Developed by LeCun, Cortes, and Burges (2010) based on two datasets from handwritten digits obtained from Census workers and high school students.

We will use only the first 500 images of the original MNIST dataset to speed up the *k-Nearest Neighbors* model's training time.

VISUALIZATION OF THE FIRST SIX IMAGES FROM THE MNIST DATA SET



HOW A IMAGE IS STORED IN THE MNIST DATASET

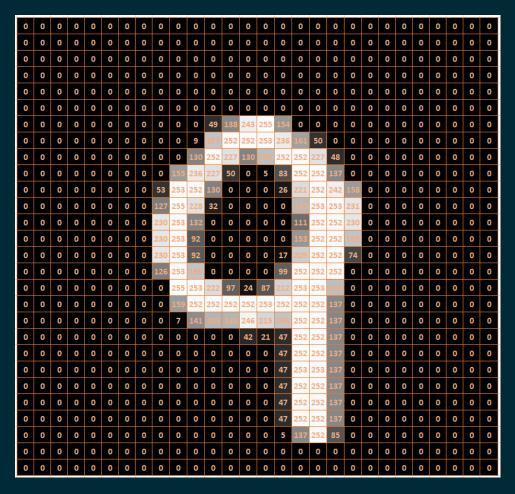
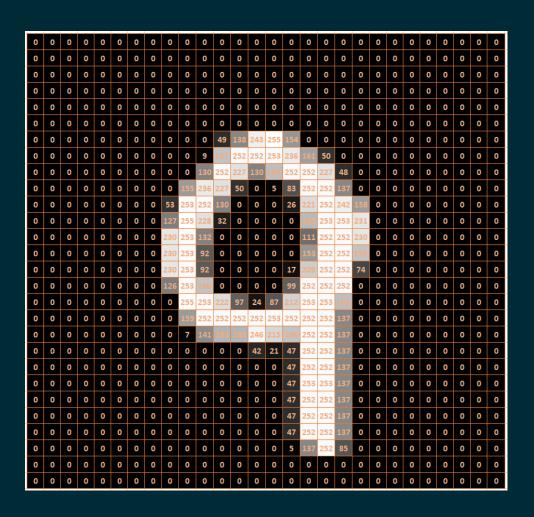


Image of a Handwritten Nine

The image has 28 rows and 28 columns. Each of the 784 cells (pixels) holds a value between 0 (black) and 255 (white)

HOW A IMAGE IS STORED IN THE MNIST DATASET



- Pixel values for a single image are not stored in a table.
 Ohterwise we would end-up with a table containing tables.
- Pixel values are stored as one row for each image.
- Concatenating the 28 rows of an image into one row with 28*28=784 cells (pixels)

Image of a Handwritten Nine

THREE ROWS FROM THE DATA FRAME OF THE MNIST DATASET

1 print(Mnist4PlotAndTable[1:3,1:784])

	Label	Pix1	Pix2 P	ix3 Pi:	x4 Pix	5 Pix6	Pix7	Pix8 P	ix9 Pi:	x10 Pi:	x11 Piz	k12 Pi	x13
	0	0	0	0	0 (0 0	0	0	0	0	0	0	0
	5	0	0	0	0 (0 0	0	0	0	0	0	0	0
3	3	0	0	0	0 (0 0	0	0	0	0	0	0	0
	Pix14	Pix15	Pix16	Pix17	Pix18	Pix19	Pix20	Pix21	Pix22	Pix23	Pix24	Pix25	Pix26
	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0
	Pix27	Pix28	Pix29	Pix30	Pix31	Pix32	Pix33	Pix34	Pix35	Pix36	Pix37	Pix38	Pix39
	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0
	Pix40	Pix41	Pix42	Pix43	Pix44	Pix45	Pix46	Pix47	Pix48	Pix49	Pix50	Pix51	Pix52
	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0
	Pix53	Pix54	Pix55	Pix56	Pix57	Pix58	Pix59	Pix60	Pix61	Pix62	Pix63	Pix64	Pix65
	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0
	Pix66	Pix67	Pix68	Pix69	Pix70	Pix71	Pix72	Pix73	Pix74	Pix75	Pix76	Pix77	Pix78
	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0
	Pix79	Pix80	Pix81	Pix82	Pix83	Pix84	Pix85	Pix86	Pix87	Pix88	Pix89	Pix90	Pix91

GO TO PROJECT IN BOOK BUILD YOUR OWN OCR SYSTEM.»