Classification I: training & predicting

Session learning objectives

By the end of the session, learners will be able to do the following:

- Recognize situations where a simple classifier would be appropriate for making predictions.
- \bullet Explain the K-nearest neighbor classification algorithm.
- Interpret the output of a classifier.
- Describe what a training data set is and how it is used in classification.
- Given a dataset with two explanatory variables/predictors, use K-nearest neighbor classification in Python using the scikit-learn framework to predict the class of a single new observation.

The classification problem

predicting a categorical class (sometimes called a *label*) for an observation given its other variables (sometimes called *features*)

- Diagnose a patient as healthy or sick
- Tag an email as "spam" or "not spam"
- Predict whether a purchase is fraudulent

Training set

Observations with known classes that we use as a basis for prediction

- Assign an observation without a known class (e.g., a new patient)
- To a class (e.g., diseased or healthy)

How?

- By similar it is to other observations for which we do know the class
 - (e.g., previous patients with known diseases and symptoms)

K-nearest neighbors

- One of many possible classification methods
 - KNN, decision trees, support vector machines (SVMs), logistic regression, neural networks, and more;

Predict observations based on other observations "close" to it

Exploring a data set

Data:

- digitized breast cancer image features, created by Dr. William H. Wolberg, W. Nick Street, and Olvi L. Mangasarian
- Each row:
 - diagnosis (benign or malignant)
 - several other measurements (nucleus texture, perimeter, area, and more)
- Diagnosis for each image was conducted by physicians.

Formulate a predictive question:

Can we use the tumor image measurements available to us to predict whether a future tumor image (with unknown diagnosis) shows a benign or malignant tumor?

Loading the cancer data

```
import pandas as pd
    import altair as alt
    cancer = pd.read csv("data/wdbc.csv")
    print(cancer)
           ID Class
                       Radius
                                Texture Perimeter
                                                        Area
                                                              Smoothness
                  M 1.096100 -2.071512
       842302
                                          1.268817 0.983510
                                                                1.567087
       842517
                  M 1.828212 -0.353322
                                        1.684473 1.907030
                                                               -0.826235
     84300903
                  M 1.578499
                              0.455786
                                          1.565126 1.557513
                                                                0.941382
566
       926954
                 M 0.701667
                              2.043775
                                        0.672084 0.577445
                                                               -0.839745
567
       927241
                  M 1.836725
                              2.334403
                                         1.980781 1.733693
                                                                1.524426
                                        -1.812793 -1.346604
568
        92751
                  B -1.806811 1.220718
                                                               -3.109349
     Compactness
                 Concavity Concave Points Symmetry
                                                      Fractal Dimension
0
       3.280628
                   2.650542
                                   2.530249 2.215566
                                                                2.253764
       -0.486643
                -0.023825
                                   0.547662 0.001391
                                                               -0.867889
       1.052000
                  1.362280
                                   2.035440
                                             0.938859
                                                               -0.397658
566
      -0.038646
                  0.046547
                                   0.105684 - 0.808406
                                                               -0.894800
       3.269267
                                                                1.042778
567
                  3.294046
                                   2.656528 2.135315
568
       -1.149741 -1.113893
                                  -1.260710 -0.819349
                                                               -0.560539
[569 rows x 12 columns]
```

these values have been standardized (centered and scaled)

Describing the variables in the cancer data set

- 1. ID: identification number
- 2. Class: the diagnosis (M = malignant or B = benign)
- 3. Radius: the mean of distances from center to points on the perimeter
- 4. Texture: the standard deviation of gray-scale values
- 5. Perimeter: the length of the surrounding contour
- 6. Area: the area inside the contour
- 7. Smoothness: the local variation in radius lengths
- 8. Compactness: the ratio of squared perimeter and area
- 9. Concavity: severity of concave portions of the contour
- 10. Concave Points: the number of concave portions of the contour
- 11. Symmetry: how similar the nucleus is when mirrored
- 12. Fractal Dimension: a measurement of how "rough" the perimeter is

DataFrame; info

```
1 cancer.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 569 entries, 0 to 568
Data columns (total 12 columns):
                        Non-Null Count Dtype
    Column
 0
                        569 non-null
                                        int64
    Class
                        569 non-null
                                        object
     Radius
                        569 non-null
                                        float64
 3
     Texture
                        569 non-null
                                        float64
                        569 non-null
                                        float64
     Perimeter
                        569 non-null
                                        float64
     Area
                        569 non-null
                                        float64
     Smoothness
                        569 non-null
                                        float64
     Compactness
                        569 non-null
                                        float64
     Concavity
     Concave Points
                        569 non-null
                                        float64
 9
    Symmetry
                        569 non-null
                                        float64
 11 Fractal Dimension 569 non-null
                                        float64
dtypes: float64(10), int64(1), object(1)
memory usage: 53.5+ KB
```

Series; unique

```
1 cancer["Class"].unique()
array(['M', 'B'], dtype=object)
```

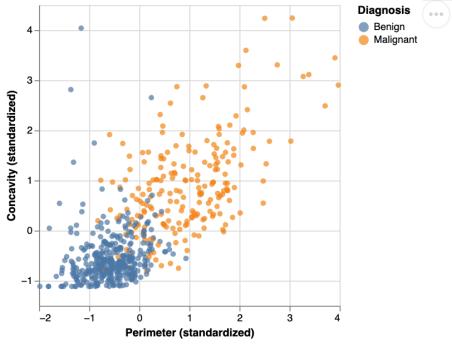
Series; replace

```
1 cancer["Class"] = cancer["Class"].replace({
2     "M" : "Malignant",
3     "B" : "Benign"
4     })
5     cancer["Class"].unique()
array(['Malignant', 'Benign'], dtype=object)
```

Exploring the cancer data

```
1 cancer.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 569 entries, 0 to 568
Data columns (total 12 columns):
                        Non-Null Count Dtype
    Column
                        569 non-null
                                        int64
 0
     TD
    Class
                        569 non-null
                                        object
                        569 non-null
     Radius
                                        float64
                        569 non-null
                                        float.64
     Texture
    Perimeter
                        569 non-null
                                        float64
                        569 non-null
                                        float64
     Area
     Smoothness
                        569 non-null
                                        float64
    Compactness
                        569 non-null
                                        float64
                        569 non-null
                                        float64
    Concavity
                                        float64
    Concave Points
 9
                        569 non-null
    Symmetry
                                        float64
                        569 non-null
11 Fractal Dimension 569 non-null
                                        float64
dtypes: float64(10), int64(1), object(1)
memory usage: 53.5+ KB
```

Visualization; scatter



- Malignant: upper right-hand corner
- Benign: lower left-hand corner

Classification with K-nearest neighbors

```
1 new point = [2, 4]
    attrs = ["Perimeter", "Concavity"]
    points df = pd.DataFrame(
        {"Perimeter": new point[0], "Concavity": new point[1], "Class": ["Unknown"]}
  6
    perim concav with new point df = pd.concat((cancer, points df), ignore index=True)
    print(perim concav with new point df.iloc[[-1]])
          Class Radius Texture Perimeter Area
                                                   Smoothness
                                                               Compactness \
569 NaN Unknown
                                         2.0
                    NaN
                              NaN
                                              NaN
                                                          NaN
                                                                        NaN
    Concavity Concave Points Symmetry Fractal Dimension
569
          4.0
                          NaN
                                     NaN
                                                        NaN
```

Compute the distance matrix between each pair from a vector array X and Y

```
from sklearn.metrics.pairwise import euclidean_distances

# distance of new point to all other points
my_distances = euclidean_distances(perim_concav_with_new_point_df[attrs])[len(cancer)][:-1]
```

Distances (euclidean_distances())

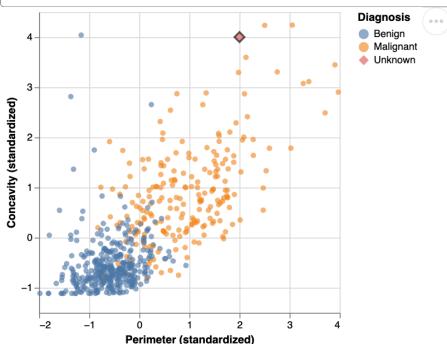
```
1 len(my distances)
569
 1 # distance of new point to all other points
 2 my distances
array([1.5348178 , 4.03617694, 2.67332814, 3.32713588, 2.63979916,
       3.93975767, 3.79946977, 4.45111808, 3.53679058, 3.24726821,
      4.951685 , 4.1538876 , 2.54585424, 4.15425044, 3.11637861,
      3.55044614, 4.59148187, 3.2419721 , 3.28753437, 4.80392314,
       5.0725937 , 5.77909213, 2.95751989, 3.74039071, 3.43925614,
      2.52875652, 3.77084705, 3.33265886, 3.38875698, 4.01548319,
      2.29844791, 4.41639587, 2.37500289, 3.07980178, 3.68423234,
       3.64538579, 3.96211289, 5.35324353, 5.15747872, 4.34753568,
      5.22721626, 4.73904767, 2.52193106, 4.45490282, 4.66689367,
      2.72752709, 6.12589249, 4.22308671, 4.99998799, 5.02870163,
      5.6046947 , 5.35214561, 5.55043261, 3.00901521, 4.79823955,
      5.48235796, 3.5095414 , 3.95297778, 5.63490804, 6.01390031,
      5.87933291, 5.91132619, 3.03871581, 5.49969602, 4.39948134,
      3.94696965, 5.86541424, 5.44232875, 3.5688574 , 5.25454378,
       3.82344861, 5.25379158, 3.18218244, 4.62286207, 5.32774445,
       4.16803695, 4.77170639, 3.116331 , 0.42493342, 5.19385448,
      5.30482795, 4.27283113, 1.5738716 , 2.72530186, 5.28695027,
      3.53135424, 4.07667556, 3.36046764, 5.02616064, 4.28105636,
      5.08987644, 4.06173178, 5.23583761, 5.12196626, 3.41101552,
       3.29340171, 5.45247337, 5.97564782, 5.33610215, 4.36938678,
      4.5747129 , 6.48184167, 5.47542661, 5.36604536, 5.613812 ,
       3.33949831, 5.01110652, 5.41189651, 0.55551675, 5.27565211,
```

K-nearest neighbors; classification

- 1. find the K "nearest" or "most similar" observations in our training set
- 2. predict new observation based on closest points

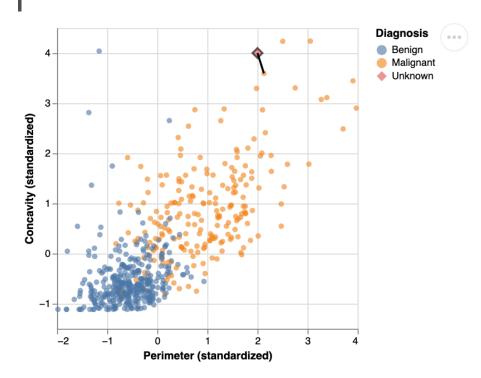
KNN Example: new point

```
perim concav with new point = (
 2
       alt.Chart(perim concav with new point df)
        .mark point(opacity=0.6, filled=True, size=40)
        .encode(
           x=alt.X("Perimeter").title("Perimeter (standardized)"),
           y=alt.Y("Concavity").title("Concavity (standardized)"),
 6
            color=alt.Color("Class").title("Diagnosis"),
            shape=alt.Shape("Class").scale(range=["circle", "circle", "diamond"]),
           size=alt.condition("datum.Class == 'Unknown'", alt.value(100), alt.value(30)),
 9
            stroke=alt.condition("datum.Class == 'Unknown'", alt.value("black"), alt.value(None)),
10
11
12
13
14 perim concav with new point
```

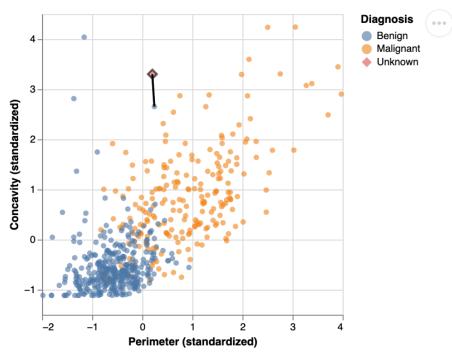


KNN example: closest point

if a point is close to another in the scatter plot, then the perimeter and concavity values are similar, and so we may expect that they would have the same diagnosis

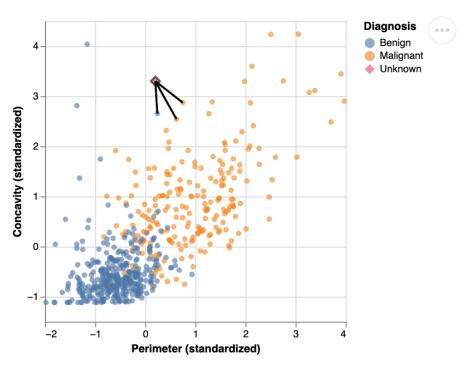


KNN Example: another new point



KNN: improve the prediction with **k**

we can consider several neighboring points, k=3

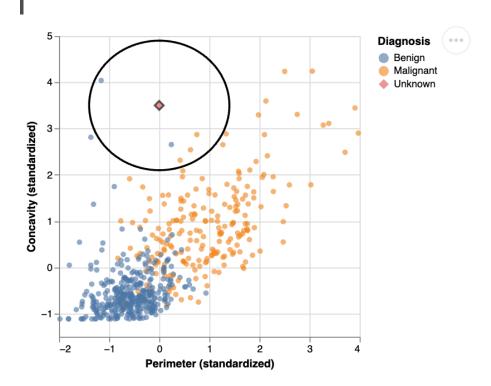


Distance between points

Distance =
$$\sqrt{(a_x - b_x)^2 + (a_y - b_y)^2}$$

Distance between points: k=5

3 of the 5 nearest neighbors to our new observation are malignant

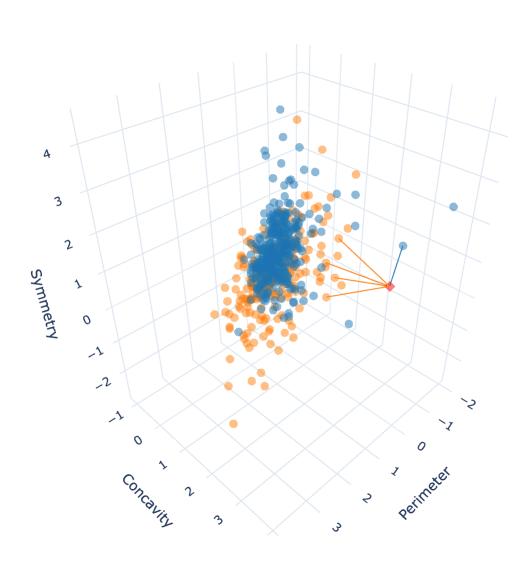


More than two explanatory variables: distance formula

The distance formula becomes

Distance =
$$\sqrt{(a_1 - b_1)^2 + (a_2 - b_2)^2 + \dots + (a_m - b_m)^2}$$
.

More than two explanatory variables: visualize



Class

- Malignant
- Benign
- Unknown

Summary of K-nearest neighbors algorithm

The K-nearest neighbors algorithm works as follows:

- 1. Compute the distance between the new observation and each observation in the training set
- 2. Find the K rows corresponding to the K smallest distances
- 3. Classify the new observation based on a majority vote of the neighbor classes

K-nearest neighbors with scikitlearn

K-nearest neighbors algorithm is implemented in scikit-learn

```
1 from sklearn import set_config
2
3 # Output dataframes instead of arrays
4 set_config(transform_output="pandas")
```

Now we can get started with sklearn and KNeighborsClassifier()

```
1 from sklearn.neighbors import KNeighborsClassifier
```

Review cancer data

```
1 cancer_train = cancer[["Class", "Perimeter", "Concavity"]]
 2 print(cancer train)
        Class Perimeter Concavity
    Malignant
                1.268817
                          2.650542
    Malignant 1.684473
                         -0.023825
    Malignant
               1.565126
                         1.362280
                               . . .
    Malignant 0.672084
566
                         0.046547
    Malignant
                1.980781
567
                         3.294046
568
       Benign -1.812793
                         -1.113893
[569 rows x 3 columns]
```

scikit-learn: Create Model Object

```
from sklearn.neighbors import KNeighborsClassifier
knn = KNeighborsClassifier(n neighbors=5)
knn
```

KNeighborsClassifier 🔍 🕜





KNeighborsClassifier()

scikit-learn: Fit the model

```
1 knn.fit(
    X=cancer train[["Perimeter", "Concavity"]],
    y=cancer train["Class"]
4 )
```

KNeighborsClassifier 🔍 🕖



KNeighborsClassifier()



- 1. We do not re-assign the variable
- 2. The arguments are X and y (note the capitalization). This comes from matrix notation.

scikit-learn: Predict

Data preprocessing: Scaling

For KNN:

- the scale of each variable (i.e., its size and range of values) matters
- distance based algorithm

Compare these 2 scenarios:

- Person A (200 lbs, 6ft tall) vs Person B (202 lbs, 6ft tall)
- Person A (200 lbs, 6ft tall) vs Person B (200 lbs, 8ft tall)

All have a distance of 2

Data preprocessing: Centering

Many other models:

- center of each variable (e.g., its mean) matters as well
- Does not matter as much in KNN:
- Person A (200 lbs, 6ft tall) vs Person B (202 lbs, 6ft tall)
- Person A (200 lbs, 6ft tall) vs Person B (200 lbs, 8ft tall)

Difference in weight is in the 10s, difference in height is fractions of a foot.

Data preprocessing: Standardization

- The mean is used to center, the standard deviation is used to scale
- Standardization: transform the data such that the mean is 0, and a standard deviation is 1

	Class	Area	Smoothness	
0	Malignant	1001.0	0.11840	
1	Malignant	1326.0	0.08474	
2	Malignant	1203.0	0.10960	
•••	•••	•••	•••	
566	Malignant	858.1	0.08455	
567	Malignant	1265.0	0.11780	
568	Benign	181.0	0.05263	

scikit-learn: ColumnTransformer

- scikit-learn has a preprocessing module
 - StandardScaler(): scale our data
- make_column_transformer: creates a ColumnTransformer to select columns

```
1 from sklearn.preprocessing import StandardScaler
 from sklearn.compose import make_column_transformer
  preprocessor = make column transformer(
      (StandardScaler(), ["Area", "Smoothness"]),
  preprocessor
```

- ColumnTransformer 1 ?
- - standardscaler
 - StandardScaler

scikit-learn: Select numeric columns

```
from sklearn.compose import make column selector
preprocessor = make column transformer(
    (StandardScaler(), make column selector(dtype_include="number")),
preprocessor
```

- ColumnTransformer 1 ?
- - standardscaler
 - StandardScaler

scikit-learn: transform

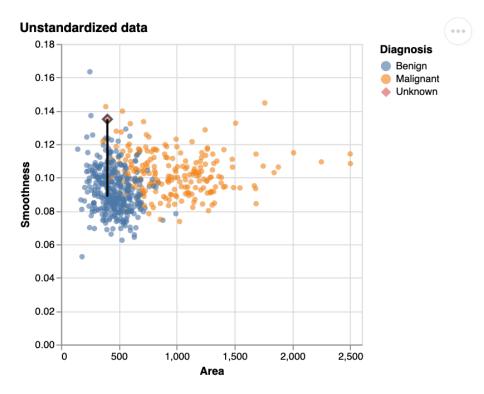
Scale the data

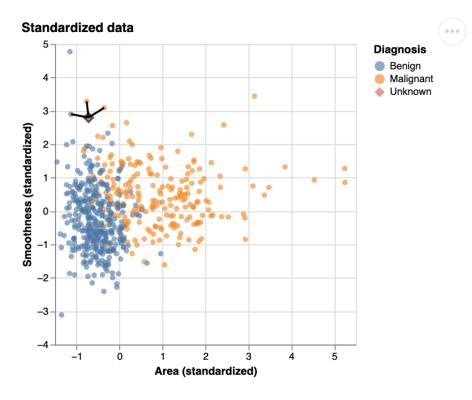
```
preprocessor.fit(unscaled_cancer)
scaled_cancer = preprocessor.transform(unscaled_cancer)
```

Compare unscaled vs scaled

1 print(unscaled_cancer)			1 print(scaled_cancer)			
	Class	Area	Smoothness		standardscalerArea	standardscalerSmoothness
0	Malignant	1001.0	0.11840	0	0.984375	1.568466
1	Malignant	1326.0	0.08474	1	1.908708	-0.826962
2	Malignant	1203.0	0.10960	2	1.558884	0.942210
• •	• • •	• • •	• • •	• •	• • •	•••
566	Malignant	858.1	0.08455	566	0.577953	-0.840484
567	Malignant	1265.0	0.11780	567	1.735218	1.525767
568	Benign	181.0	0.05263	568	-1.347789	-3.112085
[569 rows x 3 columns]			[569	[569 rows x 2 columns]		

Visualize unstandarized vs standarized data





Why scikit-learn pipelines?

- Manually standarizing is error prone
- Does not automatically account for new data
- Prevent data leakage by processing on training data to use on test data (later)
- Need same mean and standarization from training to use on test / new data

Balancing + class imbalance

21

4.546829

What if we have class imbalance? i.e., if the response variable has a big difference in frequency counts between classes?

```
rare cancer = pd.concat((
  2
        cancer[cancer["Class"] == "Benign"],
        cancer[cancer["Class"] == "Malignant"].head(3) # only 3 total
  4
    ))
    print(rare cancer)
                 Class
                          Radius
                                   Texture Perimeter
                                                           Area Smoothness \
         TD
                Benign -0.166653 -1.146154 -0.185565 -0.251735
     8510426
                                                                   0.101657
19
                Benign -0.297184 -0.832276 -0.260877 -0.383301
    8510653
                                                                  0.792066
                Benign -1.311926 -1.592558 -1.301661 -1.082620
21
     8510824
                                                                   0.429441
     842302 Malignant 1.096100 -2.071512 1.268817 0.983510
                                                                   1.567087
             Malignant 1.828212 -0.353322 1.684473 1.907030
                                                                  -0.826235
     842517
             Malignant 1.578499 0.455786
   84300903
                                             1.565126 1.557513
                                                                   0.941382
   Compactness
                Concavity
                           Concave Points
                                           Symmetry
                                                    Fractal Dimension \
     -0.436466
                -0.277965
                                -0.028584
                                           0.267676
                                                             -0.727669
19
     0.429044 - 0.540886
                                -0.459223 0.566790
20
                                                              0.752425
     -0.746429
                -0.743094
                                -0.725698
                                           0.012334
                                                              0.885562
      3.280628
                2.650542
                                 2.530249 2.215566
                                                              2.253764
     -0.486643
                -0.023825
                                 0.547662 0.001391
                                                             -0.867889
      1.052000
                1.362280
                                                             -0.397658
                                 2.035440 0.938859
   dist from new
        3.852759
19
20
        4.072405
```

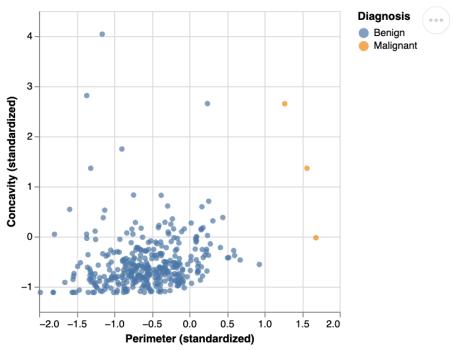
Visualizing class imbalance

```
1 rare_cancer["Class"].value_counts()
```

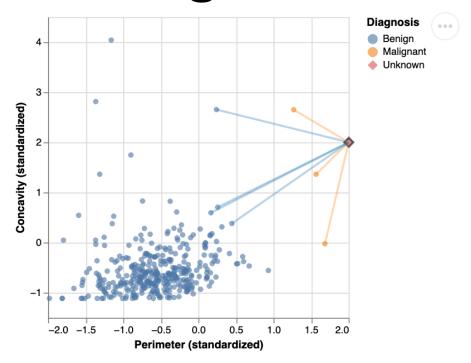
Class

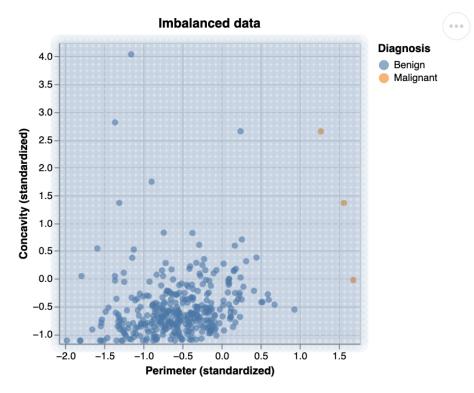
Benign 357 Malignant 3

Name: count, dtype: int64



Predicting with class imbalance





Upsampling

Rebalance the data by oversampling the rare class

- 1. Separate the classes out into their own data frames by filtering
- 2. Use the sample() method on the rare class data frame
 - Sample with replacement so the classes are the same size
- 3. Use the value_counts () method to see that our classes are now balanced

Upsampling: code

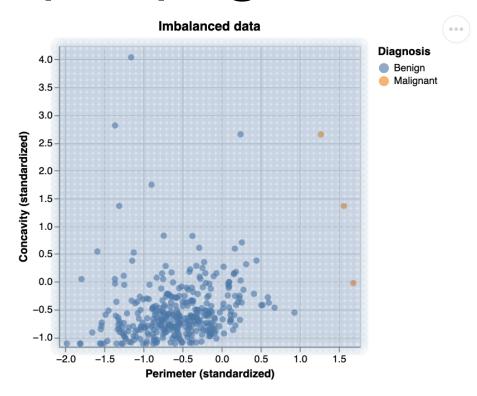
Set seed

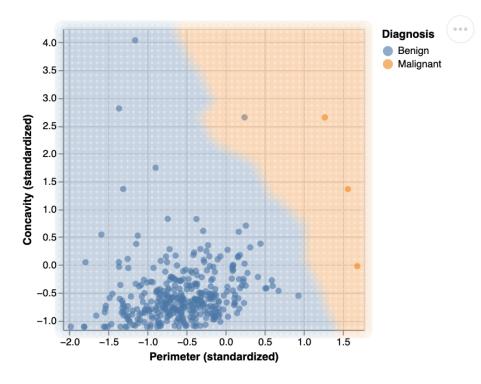
```
import numpy as np
np.random.seed(42)
```

Upsample the rare class

Class
Malignant 357
Benign 357
Name: count, dtype: int64

Upsampling: Re-train KNN k=7





Missing data

Assume we are only looking at "randomly missing" data

```
Texture Perimeter
      Class
               Radius
                                1.268817
  Malignant
                 NaN
                           NaN
1 Malignant 1.828212 -0.353322
                               1.684473
2 Malignant 1.578499
                           NaN
                                1.565126
3 Malignant -0.768233 0.253509
                               -0.592166
4 Malignant 1.748758 -1.150804
                               1.775011
 Malignant -0.475956 -0.834601
                               -0.386808
  Malignant 1.169878 0.160508
                                1.137124
```

Missing data: .dropna()

KNN computes distances across all the features, it needs complete observations

```
1  # drop incomplete observations
2  no_missing_cancer = missing_cancer.dropna()
3  print(no_missing_cancer)

Class    Radius    Texture    Perimeter
1  Malignant    1.828212    -0.353322     1.684473
3  Malignant    -0.768233     0.253509     -0.592166
4  Malignant    1.748758    -1.150804     1.775011
5  Malignant    -0.475956    -0.834601     -0.386808
6  Malignant    1.169878     0.160508     1.137124
```

Missing data: SimpleImputer()

We can impute missing data (with the mean) if there's too many missing values

```
from sklearn.impute import SimpleImputer
preprocessor = make column transformer(
    (SimpleImputer(), ["Radius", "Texture", "Perimeter"]),
    verbose feature names out=False,
preprocessor
```

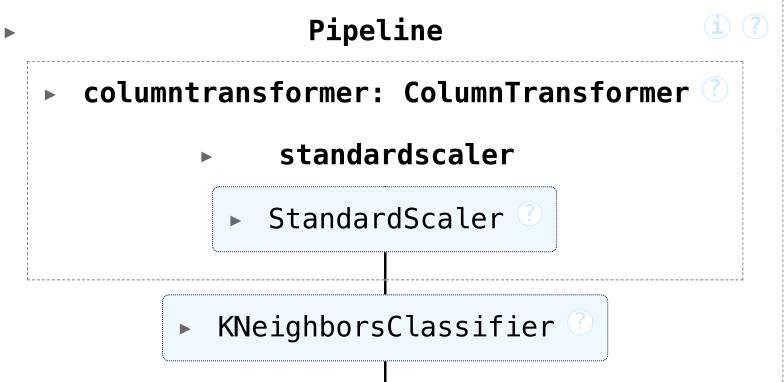
- ColumnTransformer 1 ?
- - simpleimputer
 - SimpleImputer

Imputed data

```
preprocessor.fit(missing cancer)
  imputed cancer = preprocessor.transform(missing cancer)
1 print(missing cancer)
                                                        1 print(imputed cancer)
             Radius
                      Texture Perimeter
                                                           Radius
                                                                    Texture Perimeter
    Class
Malignant
                NaN
                               1.268817
                                                      0 0.846860 -0.384942
                                                                             1.268817
                          NaN
Malignant 1.828212 -0.353322
                               1.684473
                                                      1 1.828212 -0.353322
                                                                             1.684473
Malignant 1.578499
                               1.565126
                                                      2 1.578499 -0.384942
                                                                             1.565126
                          NaN
Malignant -0.768233
                    0.253509
                              -0.592166
                                                      3 -0.768233 0.253509 -0.592166
Malignant 1.748758 -1.150804
                              1.775011
                                                      4 1.748758 -1.150804
                                                                            1.775011
Malignant -0.475956 -0.834601
                              -0.386808
                                                      5 -0.475956 -0.834601 -0.386808
Malignant 1.169878 0.160508
                               1.137124
                                                      6 1.169878 0.160508
                                                                             1.137124
```

Put it all together: Preprocessor

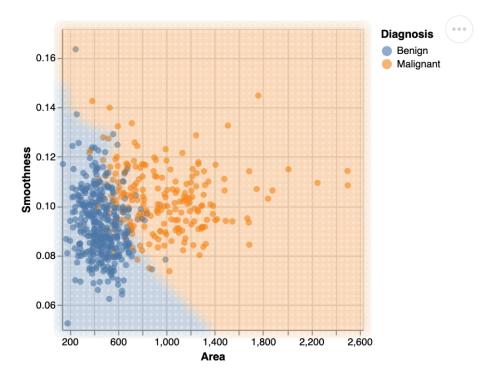
Put it all together: Pipeline



Put it all together: Predict

Prediction Area

Model prediction area.



- Points are on original unscaled data
- Area is using the pipeline model

Reference Code

```
import pandas as pd
 2 from sklearn.preprocessing import StandardScaler
 3 from sklearn.neighbors import KNeighborsClassifier
   from sklearn.pipeline import make pipeline
   from sklearn.compose import (
       make column transformer,
 6
 8
   # load the unscaled cancer data
   unscaled cancer = pd.read csv(
       "data/wdbc unscaled.csv"
12
13
14
   # make Class readable
   unscaled cancer["Class"] = unscaled cancer[
        "Class"
17
   ].replace({"M": "Malignant", "B": "Benign"})
```

```
1 # create the K-NN model
   knn = KNeighborsClassifier(n neighbors=7)
   # create the centering / scaling preprocessor
   preprocessor = make column transformer(
       (StandardScaler(), ['Area', 'Smoothness']),
       # more column transformers here
 8
 9
   knn pipeline = make pipeline(preprocessor, knn)
   knn pipeline.fit(X=unscaled cancer, y=unscaled can
   knn pipeline
13
   new observation = pd.DataFrame(
15
            'Area': [500, 1500],
16
            'Smoothness': [0.075, 0.1],
17
18
19
   prediction = knn pipeline.predict(new observation)
21 prediction
```

array(['Benign', 'Malignant'], dtype=object)

Additional resources

- The Classification I: training & predicting chapter of Data Science: A First
 Introduction (Python Edition) by Tiffany Timbers, Trevor Campbell, Melissa Lee, Joel
 Ostblom, Lindsey Heagy contains all the content presented here with a detailed
 narrative.
- The scikit-learn website is an excellent reference for more details on, and advanced usage of, the functions and packages in this lesson. Aside from that, it also offers many useful tutorials to get you started.
- An Introduction to Statistical Learning by Gareth James Daniela Witten Trevor Hastie, and Robert Tibshirani provides a great next stop in the process of learning about classification. Chapter 4 discusses additional basic techniques for classification that we do not cover, such as logistic regression, linear discriminant analysis, and naive Bayes.

References

Lars Buitinck, Gilles Louppe, Mathieu Blondel, Fabian Pedregosa, Andreas Mueller, Olivier Grisel, Vlad Niculae, Peter Prettenhofer, Alexandre Gramfort, Jaques Grobler, Robert Layton, Jake VanderPlas, Arnaud Joly, Brian Holt, and Gaël Varoquaux. API design for machine learning software: experiences from the scikit-learn project. In ECML PKDD Workshop: Languages for Data Mining and Machine Learning, 108–122. 2013.

Thomas Cover and Peter Hart. Nearest neighbor pattern classification. IEEE Transactions on Information Theory, 13(1):21–27, 1967.

Evelyn Fix and Joseph Hodges. Discriminatory analysis. nonparametric discrimination: consistency properties. Technical Report, USAF School of Aviation Medicine, Randolph Field, Texas, 1951.

William Nick Street, William Wolberg, and Olvi Mangasarian. Nuclear feature extraction for breast tumor diagnosis. In International Symposium on Electronic Imaging: Science and Technology. 1993.

Stanford Health Care. What is cancer? 2021. URL: https://stanfordhealthcare.org/medical-conditions/cancer/cancer.html.