TP6. Decision trees - Classification

EX.1 - Using Decision Trees to Diagnose Breast Cancer

Now that we have built our first decision trees, it's time to turn our attention to a real dataset: The Breast Cancer Wisconsin dataset https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic).

In order to make the take feasible, the researchers performed feature extraction on the images, like we did in Chapter 4, Representing Data and Engineering Features. They went through a total of 569 images, and extracted 30 different features that describe the characteristics of the cell nuclei present in the images, including:

- cell nucleus texture (represented by the standard deviation of the gray-scale values)
- cell nucleus size (calculated as the mean of distances from center to points on the perimeter)
- tissue smoothness (local variation in radius lengths)
- tissue compactness

The goal of the research was then to classify tissue samples into benign and malignant (a binary classification task).

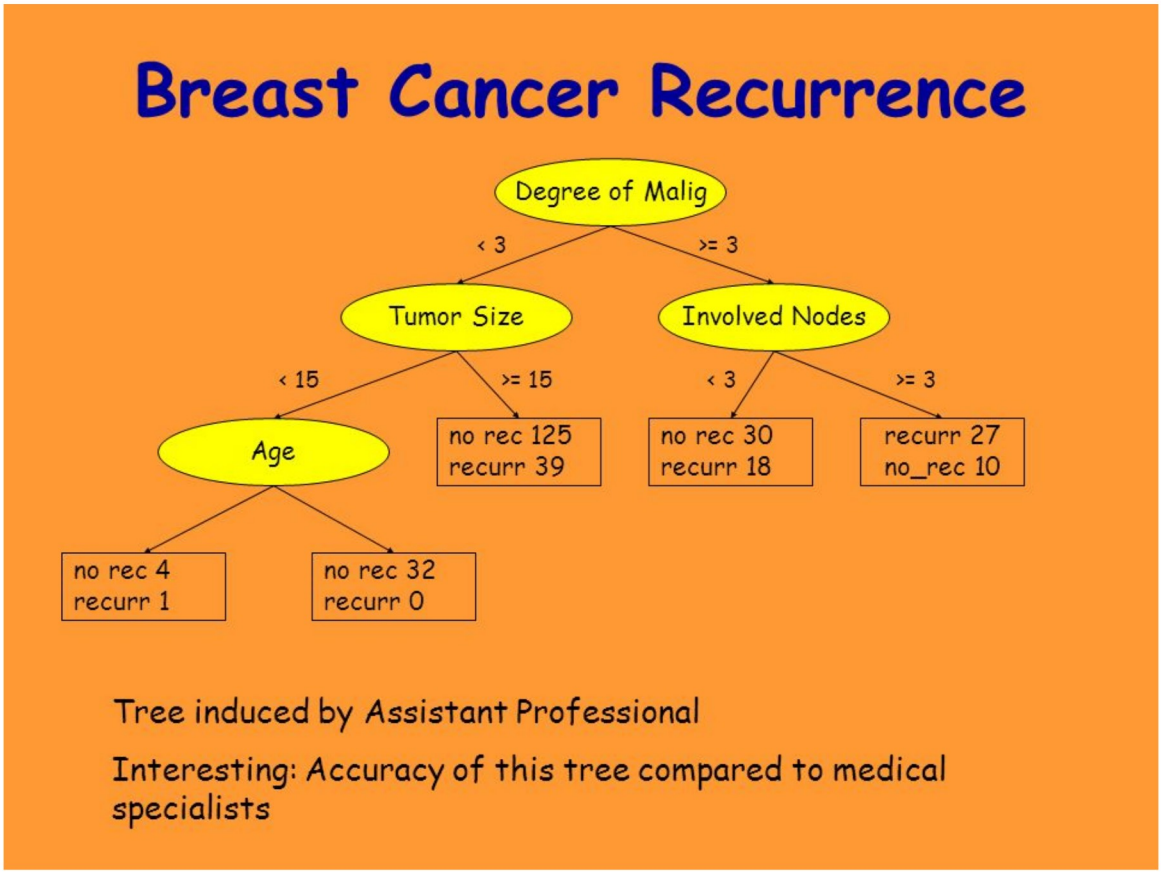
Decision trees for Classification

- the target variable uses a discrete set of values
- each node, or leaf, represent class labels while the branches represent conjunctions of features leading to class labels

In [133…

```
from IPython.display import Image
Image(filename = "tree_example.jpg", width = 600, height = 300)

#https://www.kaggle.com/code/nisasoylu/decision-tree-implementation-on-cancer-da
```

Out[133]:



a) Loading the dataset

The full dataset is part of Scikit-Learn's example datasets:

In [134…

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

#from sklearn import datasets
# read the dataset
#df=pd.read_csv('Breastcancer.csv', index_col=0)
df=pd.read_csv('Breastcancer.csv')
df.head()
```

Out[134]:

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_ı
0	842302	M	17.99	10.38	122.80	1001.0	0.1
1	842517	M	20.57	17.77	132.90	1326.0	0.(
2	84300903	M	19.69	21.25	130.00	1203.0	0.1
3	84348301	M	11.42	20.38	77.58	386.1	0.1
4	84358402	M	20.29	14.34	135.10	1297.0	0.1

5 rows × 33 columns

As in previous examples, all data is contained in a 2-D feature matrix data.data, where the rows represent data samples, and the columns are the feature values:

In [135…
```
df.shape
```

Out[135]:
```
(569, 33)
```

In [136…
```
#df.dtypes
```

In [137…
```
#checking missing values
df.isnull().sum()
```

Out[137]:
```
id                         0
diagnosis                  0
radius_mean                0
texture_mean               0
perimeter_mean             0
area_mean                  0
smoothness_mean            0
compactness_mean           0
concavity_mean             0
concave points_mean        0
symmetry_mean              0
fractal_dimension_mean     0
radius_se                  0
texture_se                 0
perimeter_se               0
area_se                    0
smoothness_se              0
compactness_se             0
concavity_se               0
concave points_se          0
symmetry_se                0
fractal_dimension_se       0
radius_worst               0
texture_worst              0
perimeter_worst            0
area_worst                 0
smoothness_worst           0
compactness_worst          0
concavity_worst            0
concave points_worst       0
symmetry_worst             0
fractal_dimension_worst    0
Unnamed: 32                569
dtype: int64
```

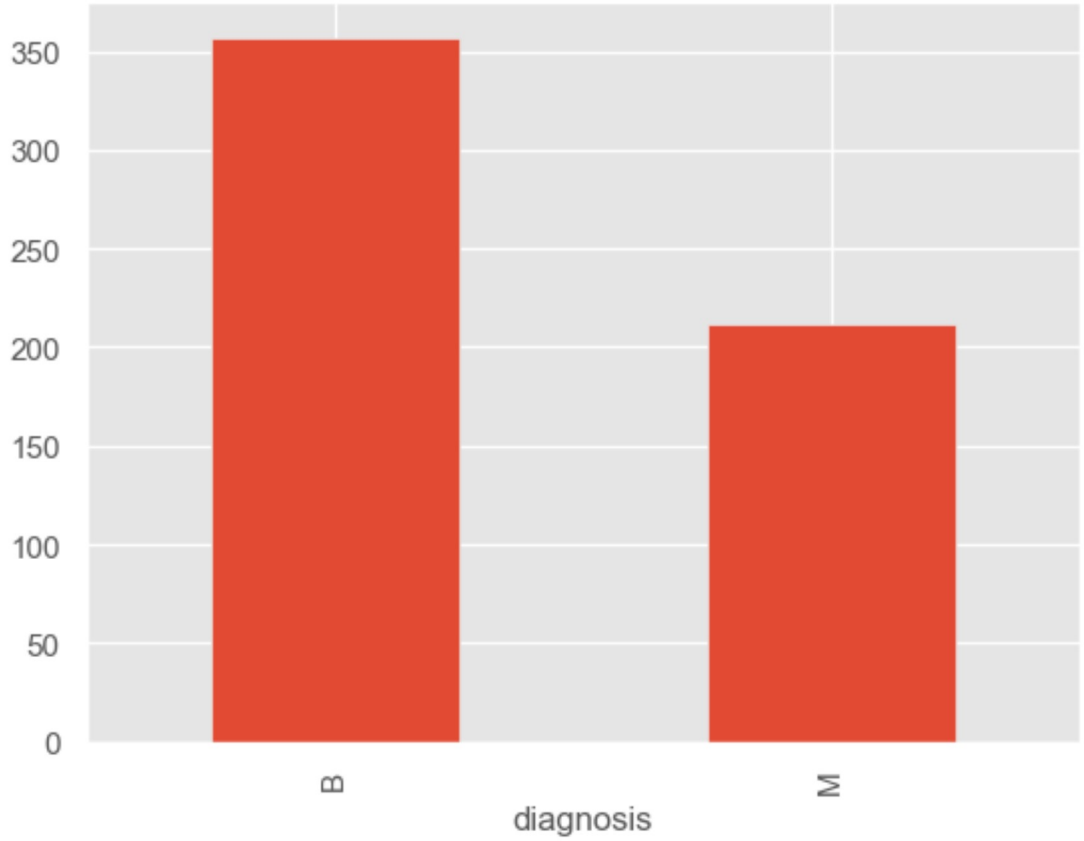
b) EDA

With a look at the provided feature names, we recognize some that we mentioned above:

Since this is a binary classification task, we expect to find exactly two target names:

In [138…
```
df.diagnosis.value_counts().plot.bar()
```

Out[138]:
```
<Axes: xlabel='diagnosis'>
```



In [139…

```
import plotly.express as px
fig = px.pie(df, values='radius_mean', names='diagnosis', title='Relation')
fig.show()
```

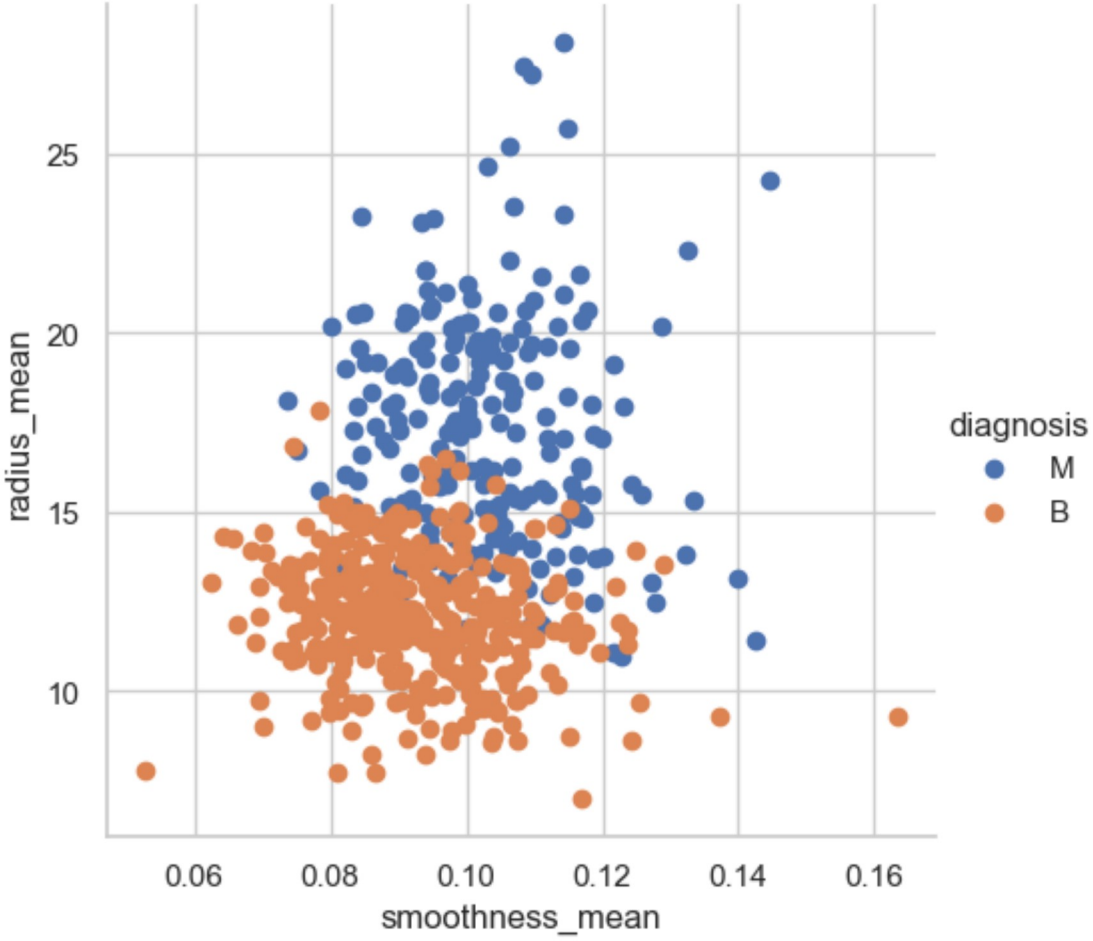
In [140…

```
import seaborn as sns
sns.set(style="whitegrid", color_codes=True)

sns.lmplot(y='radius_mean', x='smoothness_mean', hue='diagnosis',
           data=df,
           fit_reg=False, scatter_kws={'alpha':1})
```

```
C:\Users\ElsaFG\anaconda3\envs\islp\Lib\site-packages\seaborn\axisgrid.py:118: U
serWarning:

The figure layout has changed to tight
```

Out[140]:

```
<seaborn.axisgrid.FacetGrid at 0x20b7d14f190>
```

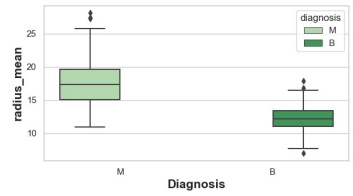


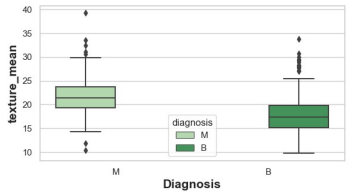
In [141…

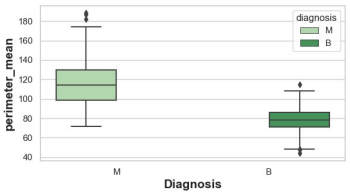
```
#Retirar a coluna do id e da Unnamed: 32, cujos gráficos não fazem sentido

df=df.drop(["id","Unnamed: 32"],axis=1)
```

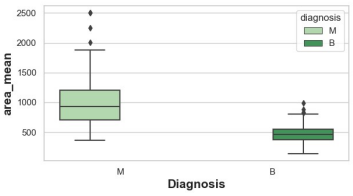
In [142…

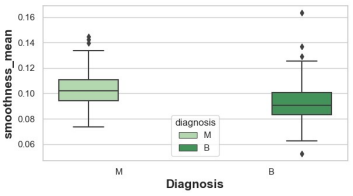
```
fig, ax = plt.subplots(10, 3, figsize=(20, 40))
ax = ax.flatten()

for i, col in enumerate(df.columns[1:]):
    #sns.boxplot(x='diagnosis', y=col, data=df, ax=ax[i], palette='Greens', hue=
    sns.boxplot(x='diagnosis', y=col, data=df, ax=ax[i], palette='Greens', hue='
    ax[i].set_xlabel('Diagnosis', fontsize = 15, fontweight = 'bold')
    ax[i].set_ylabel(col, fontsize = 15, fontweight = 'bold')

plt.tight_layout(w_pad=5, h_pad=5)
plt.show()
```

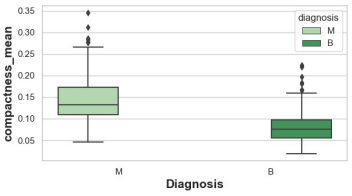

radius_mean
diagnosis
M
B
Diagnosis

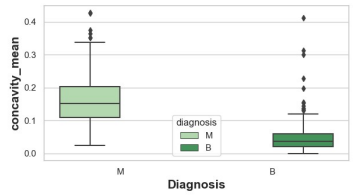

texture_mean
diagnosis
M
B
Diagnosis

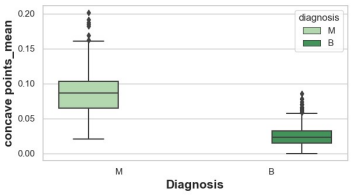

perimeter_mean
diagnosis
M
B
Diagnosis

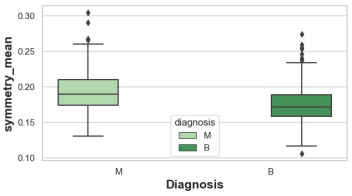

area_mean
diagnosis
M
B
Diagnosis

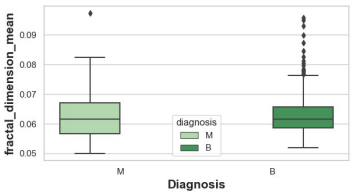

smoothness_mean
diagnosis
M
B
Diagnosis

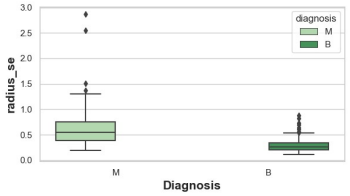

compactness_mean
diagnosis
M
B
Diagnosis

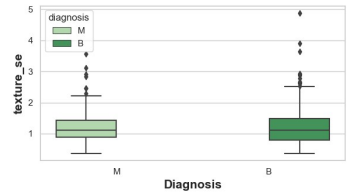

concavity_mean
diagnosis
M
B
Diagnosis

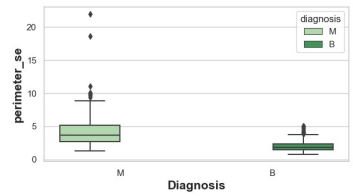

concave points_mean
diagnosis
M
B
Diagnosis

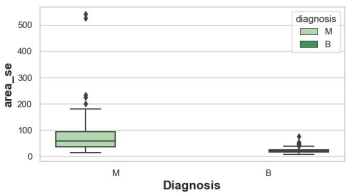

symmetry_mean
diagnosis
M
B
Diagnosis

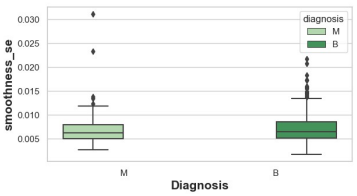

fractal_dimension_mean
diagnosis
M
B
Diagnosis

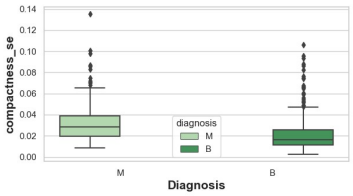

radius_se
diagnosis
M
B
Diagnosis

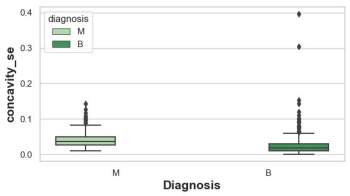

texture_se
diagnosis
M
B
Diagnosis

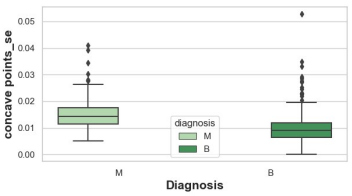

perimeter_se
diagnosis
M
B
Diagnosis

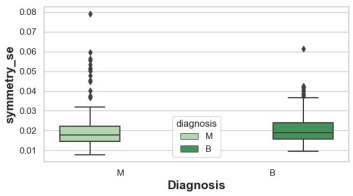

area_se
diagnosis
M
B
Diagnosis

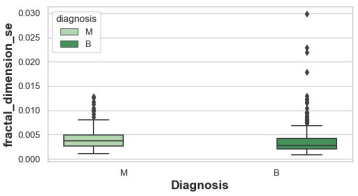

smoothness_se
diagnosis
M
B
Diagnosis

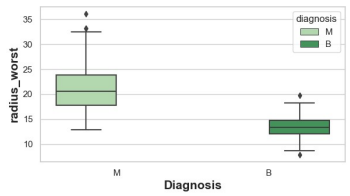

compactness_se
diagnosis
M
B
Diagnosis

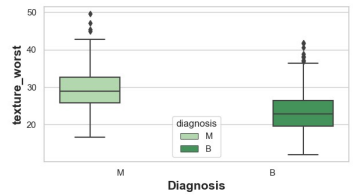

concavity_se
diagnosis
M
B
Diagnosis

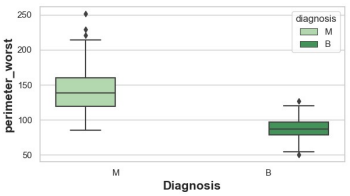

concave points_se
diagnosis
M
B
Diagnosis

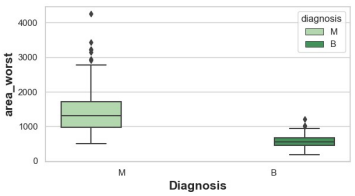

symmetry_se
diagnosis
M
B
Diagnosis

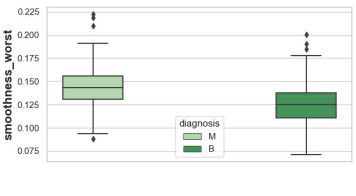

fractal_dimension_se
diagnosis
M
B
Diagnosis

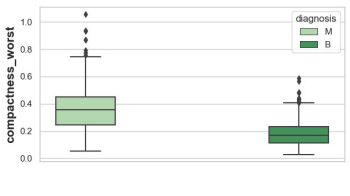

radius_worst
diagnosis
M
B
Diagnosis

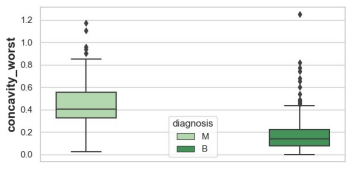

texture_worst
diagnosis
M
B
Diagnosis

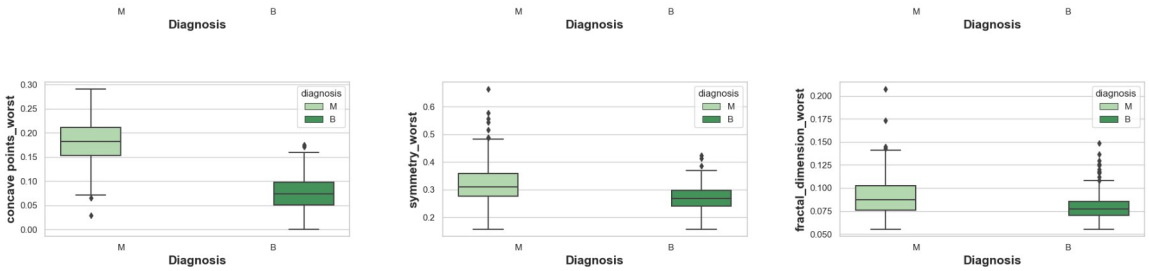

perimeter_worst
diagnosis
M
B
Diagnosis


area_worst
diagnosis
M
B
Diagnosis


smoothness_worst
diagnosis
M
B
Diagnosis

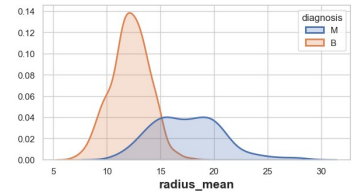

compactness_worst
diagnosis
M
B
Diagnosis

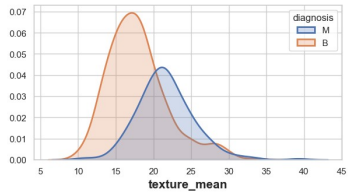

concavity_worst
diagnosis
M
B
Diagnosis

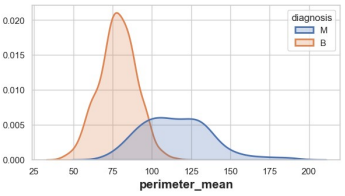


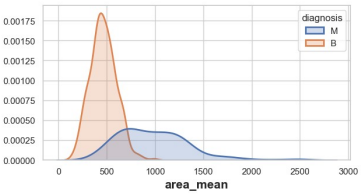
In [143…

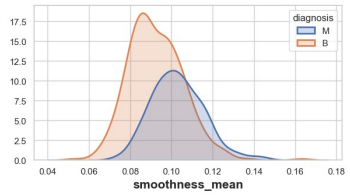
```
fig, ax = plt.subplots(10, 3, figsize=(20, 40))
ax = ax.flatten()

for i, col in enumerate(df.columns[1:]):
    sns.kdeplot(x=col, data=df, ax=ax[i], fill=True, lw=2, hue = 'diagnosis')
    ax[i].set_xlabel(col, fontsize = 15, fontweight = 'bold')
    ax[i].set_ylabel('')

plt.tight_layout(w_pad=5, h_pad=5)
plt.show()
```

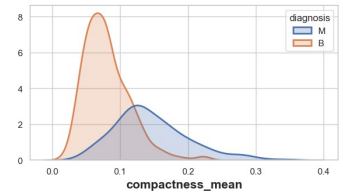

diagnosis
M
B
radius_mean

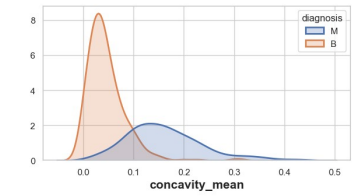

diagnosis
M
B
texture_mean

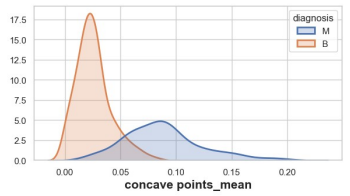

diagnosis
M
B
perimeter_mean

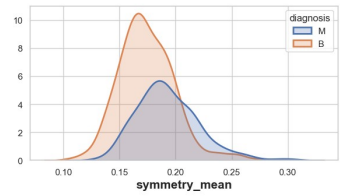

diagnosis
M
B
area_mean

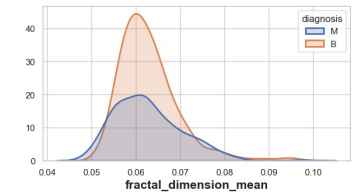

diagnosis
M
B
smoothness_mean

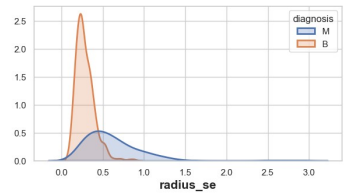

diagnosis
M
B
compactness_mean

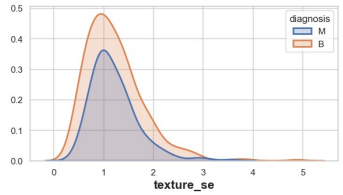

diagnosis
M
B
concavity_mean

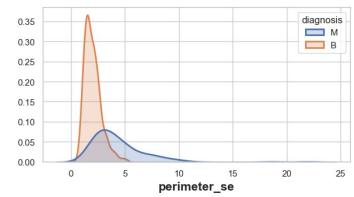

diagnosis
M
B
concave points_mean

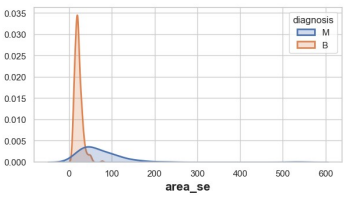

diagnosis
M
B
symmetry_mean

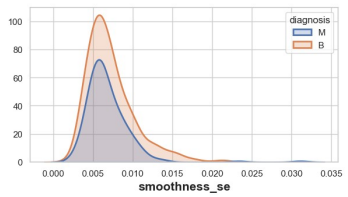

diagnosis
M
B
fractal_dimension_mean

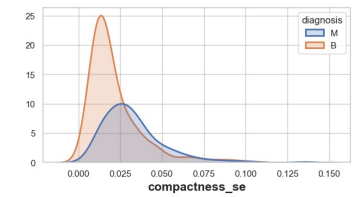

diagnosis
M
B
radius_se

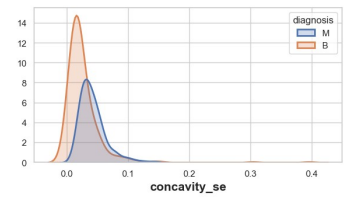

diagnosis
M
B
texture_se

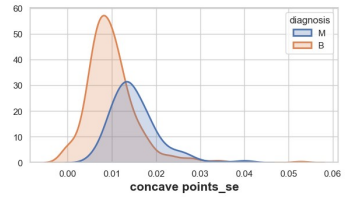

diagnosis
M
B
perimeter_se

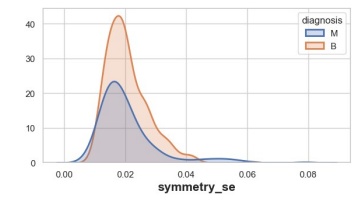

diagnosis
M
B
area_se

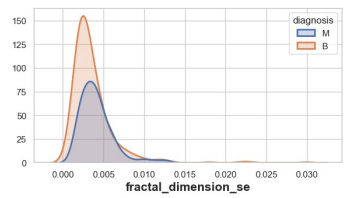

diagnosis
M
B
smoothness_se

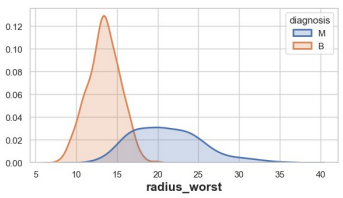

diagnosis
M
B
compactness_se

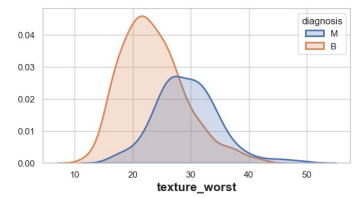

diagnosis
M
B
concavity_se

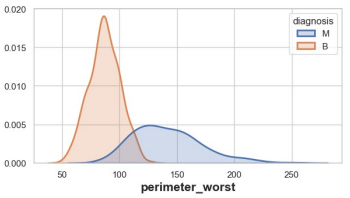

diagnosis
M
B
concave points_se

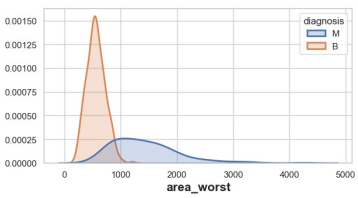

diagnosis
M
B
symmetry_se

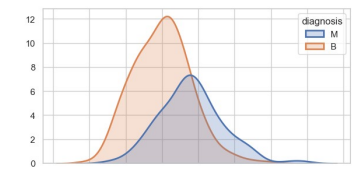

diagnosis
M
B
fractal_dimension_se

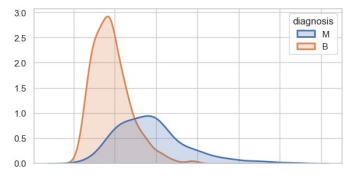

diagnosis
M
B
radius_worst


diagnosis
M
B
texture_worst

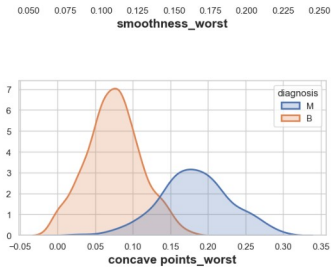

diagnosis
M
B
perimeter_worst

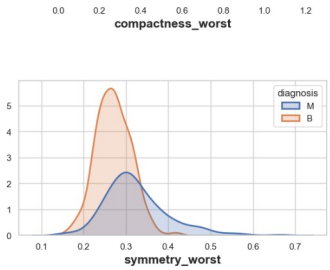

diagnosis
M
B
area_worst

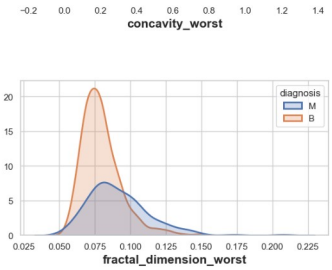

diagnosis
M
B


diagnosis
M
B


diagnosis
M
B







c) Holdout: split the dataset into training and test sets using a 70-30 split:

Data preparation

In [144…

```
#target variable
y = df.loc[:,"diagnosis"].values
#feature variable
X = df.drop(["diagnosis"],axis=1).values
```

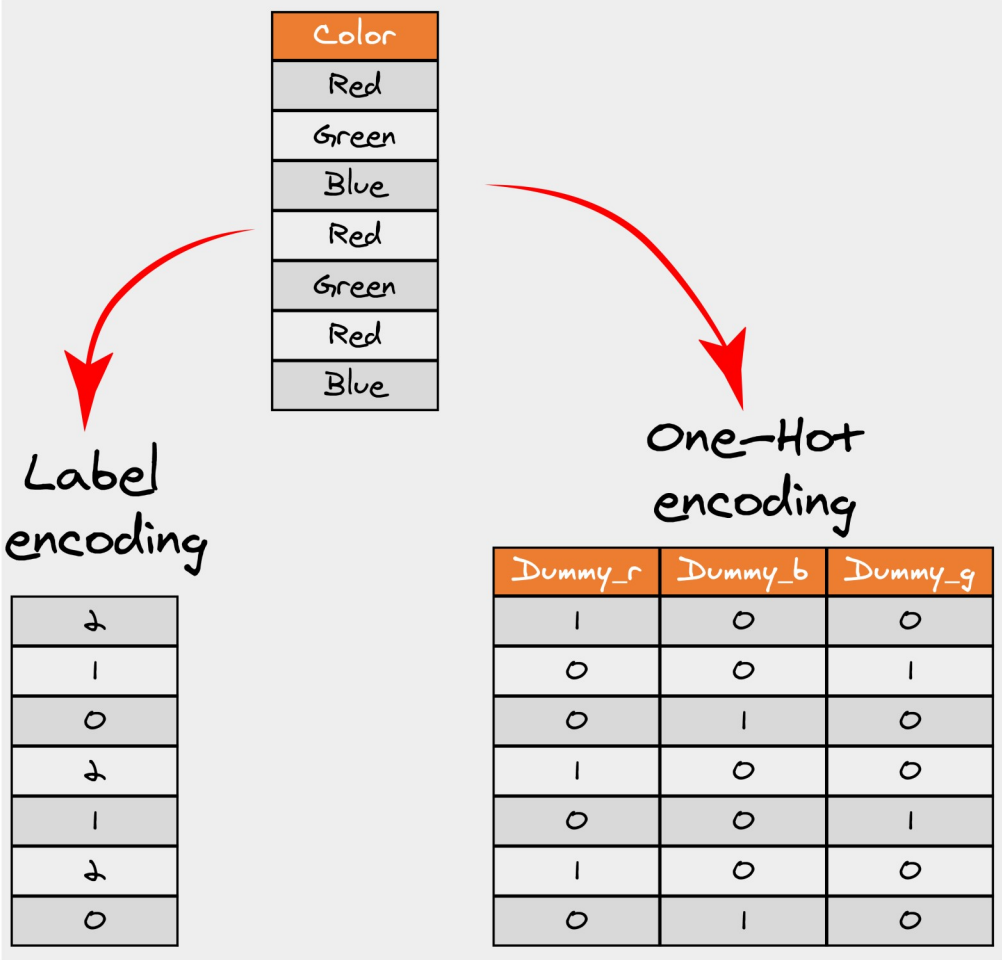
In [145…

```
# our target variable has two categories, M and B. Scikit-learn likes to work wi
#Let's encode the target variable with label encoder.
#Hint: This transformer should be used to encode target values, i.e. y, and not

from sklearn.preprocessing import LabelEncoder

le = LabelEncoder()

#fit and transform the target variable
y = le.fit_transform(y)
```

In [183…

```
from IPython.display import Image
Image(filename = "Label_encod.png", width = 500, height = 300)

#Pandas: import pandas as pd; pd.get_dummies()
#Sklearn: from sklearn.preprocessing import OneHotEncoder; OneHotEncoder()
```

Out[183]:



In [147…

```
#train and test split
from sklearn.model_selection import train_test_split

X_train,X_test,y_train,y_test=train_test_split(X,y,test_size=0.3,random_state=12
```

In [148…

```
X_train.shape, X_test.shape
```

Out[148]:

```
((398, 30), (171, 30))
```

In [150…

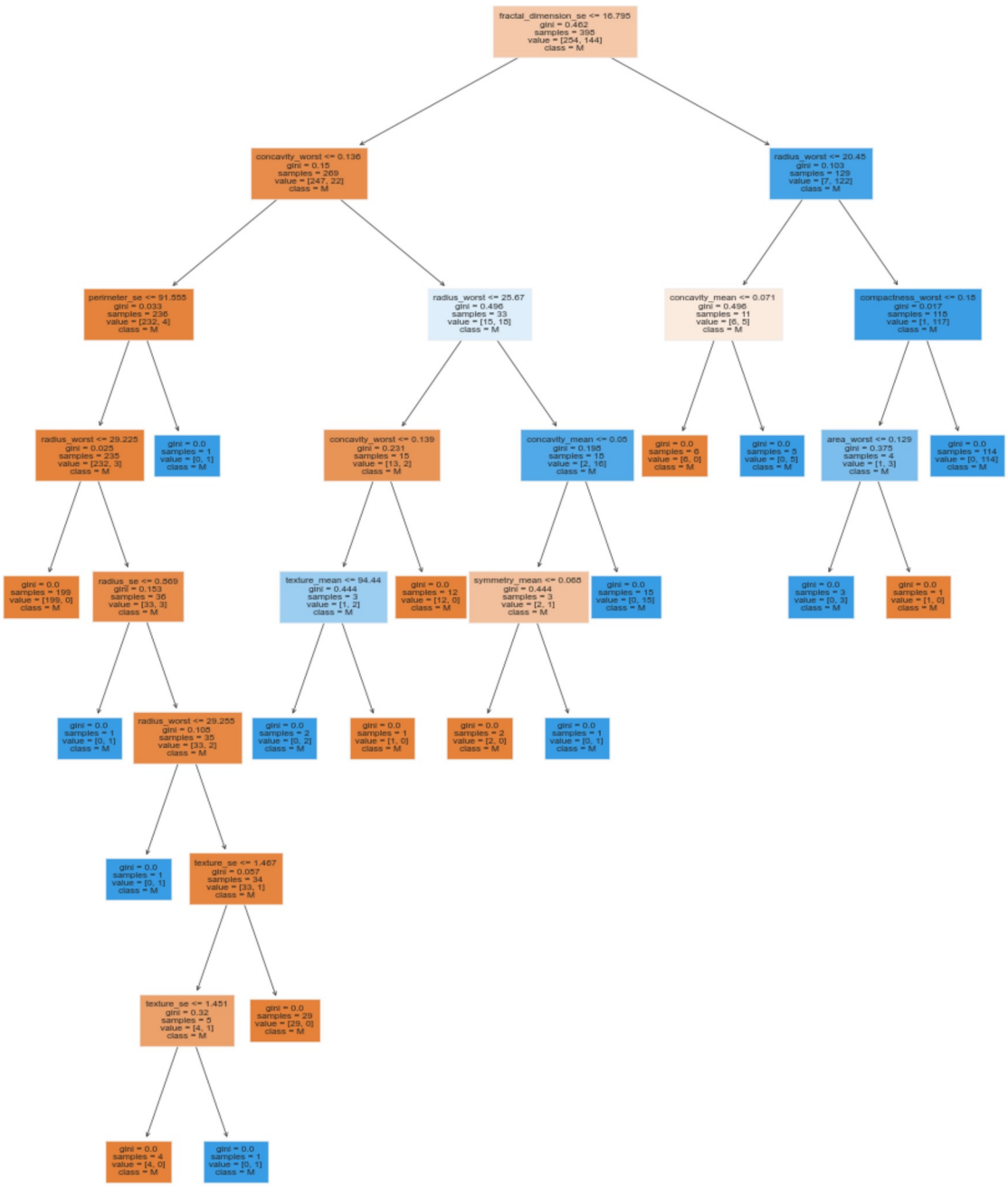
```
#Building the decision tree model

from sklearn.tree import DecisionTreeClassifier
clf = DecisionTreeClassifier(random_state = 42)

#build the model with training sets
clf.fit(X_train, y_train)

# com scale
# model = dt.fit(scaler.transform(X_train), y_train)
```

Out[150]:

```
▾        DecisionTreeClassifier

DecisionTreeClassifier(random_state=42)
```

In [151…

```
# tree visualization

from matplotlib import pyplot as plt
from sklearn.tree import plot_tree, export_text
from IPython.display import Image, display
%matplotlib inline
plt.style.use('ggplot')

# plot tree
plt.figure(figsize=(12,15))  # set plot size (denoted in inches)
plot_tree(clf,
          feature_names = list(df.columns),
          class_names = list(df['diagnosis']),
          filled=True,
          fontsize=6);
```



Since we did not specify any pre-pruning parameters, we would expect this decision tree to grow quite large and result in a perfect score on the training set:

In [152…
```
clf.score(X_train, y_train)
```

Out[152]:
```
1.0
```

However, to our surprise, the test error is not too shabby, either:

In [153…
```
clf.score(X_test, y_test)
```

Out[153]:
```
0.9649122807017544
```

In [154…
```
# Let's predict the training and the test values with this model.

y_train_pred=clf.predict(X_train)
y_test_pred=clf.predict(X_test)
```

In [155…
```
#Let's take a look at the performance of the model on the training and test set.
#To do this, we can use the accuracy_score function.

from sklearn.metrics import accuracy_score

tree_train = accuracy_score(y_train, y_train_pred)
print("Train Accuracy:", tree_train)

tree_test = accuracy_score(y_test, y_test_pred)
print("Test Accuracy:", tree_test)
```

```
Train Accuracy: 1.0
Test Accuracy: 0.9649122807017544
```

In [156…
```
# Lets also get the training error rate of the tree model
from sklearn.metrics import confusion_matrix

cmatrix = confusion_matrix(y_true = y_train, y_pred=clf.predict(X_train), labels
print(cmatrix)

error_rate = (cmatrix[0,1]+cmatrix[1,0])/cmatrix.sum()
print("Training Error Rate:", error_rate)
```

```
[[144   0]
 [  0 254]]
Training Error Rate: 0.0
```

In [157…
```
# Lets compute the error rate of the tree model

ypred = clf.predict(X_test)
cmatrix = confusion_matrix(y_true=y_test, y_pred=ypred, labels=[True, False])
print(cmatrix)
error_rate_test = (cmatrix[0,1]+cmatrix[1,0])/cmatrix.sum()
print("Test Error Rate:", error_rate_test)
```

```
[[ 64   4]
 [  2 101]]
Test Error Rate: 0.03508771929824561
```

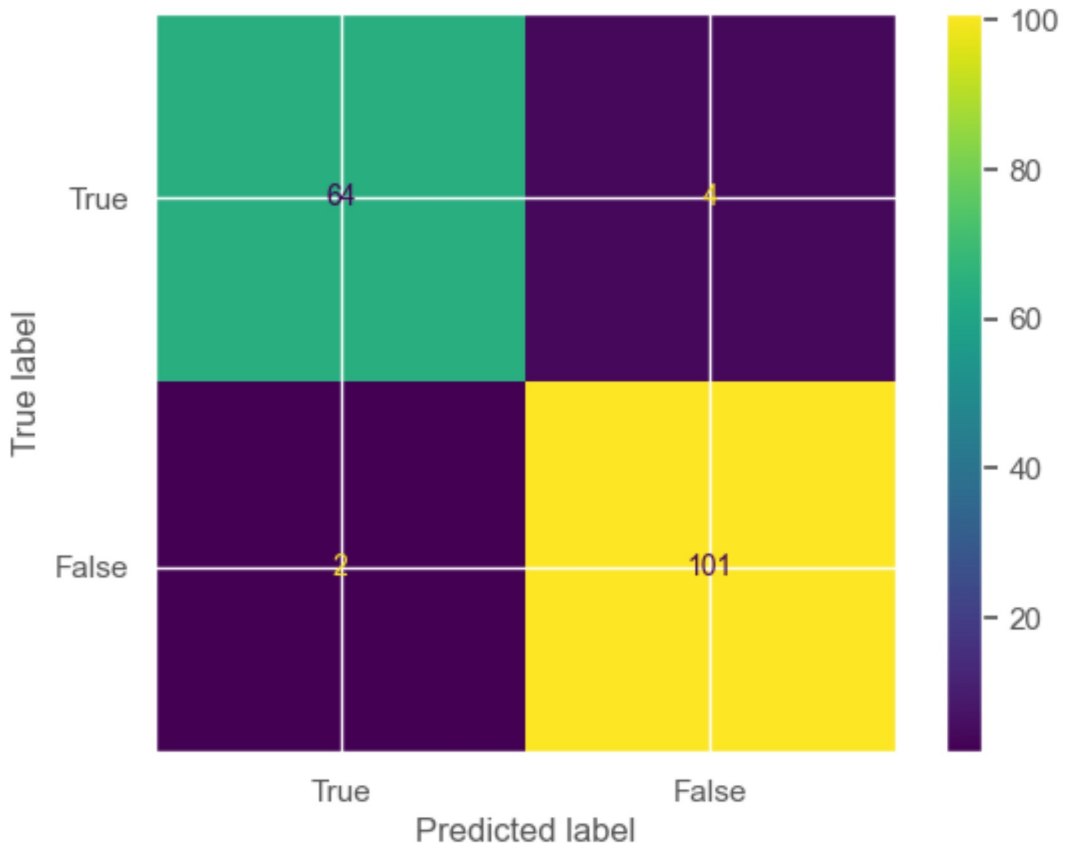
d) Confusion matrix

In [158…

```
from sklearn.metrics import ConfusionMatrixDisplay, accuracy_score

disp = ConfusionMatrixDisplay(confusion_matrix=cmatrix, display_labels=[True, Fa
disp.plot()

accuracy_score(y_test,ypred)
```

Out[158]:

```
0.9649122807017544
```



f) Confusion matrix implementation - matriz_confusao(actual, predicted)

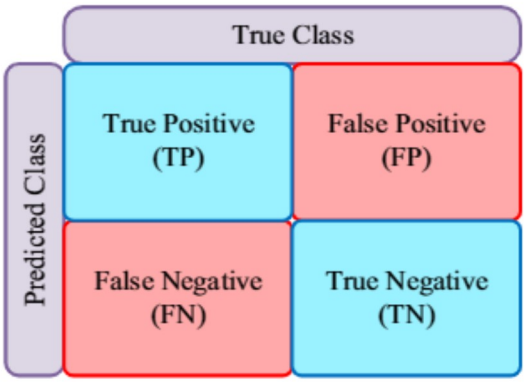
Para calcular a matriz de confusão para um problema de classificação 2-classes:

- True positives (TP): O número de casos corretamente classificados para a classe positiva.
- True negatives (TN): O número de casos corretamente classificados para a classe negativa.
- False positives (FP): O número de casos incorretamente classificados para a classe positiva.
- False negatives (FN): O número de casos incorretamente classificados para a classe negativa.

In [159…

```
## Metrics - 2 classes

Image(filename = "matriz_conf_metricas.png", width = 600, height = 300)
```

Out[159]:



Function Name	Formula
Accuracy	$\frac{TP+TN}{TP+TN+FP+FN}$
Precision	$\frac{TP}{TP+FP}$
Recall	$\frac{TP}{TP+FN}$
F1 score	$\frac{2.Precision.Recall}{Precision+Recall}$

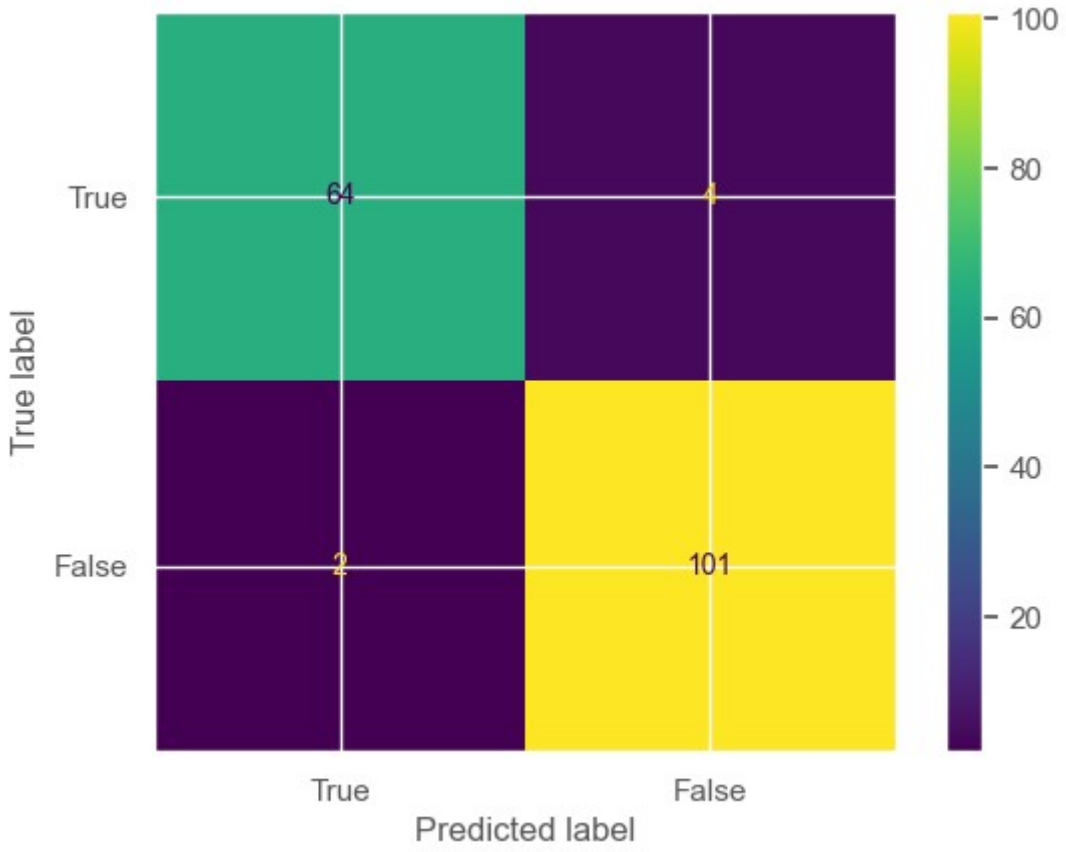
Metrics for Performance Evaluation (Medidas de desempenho)

- Accuracy: Rate of correct examples (out of total examples)
- Error rate: Rate of wrong examples (out of total examples)
- Precision: rate of positive examples classified correctly, among all predicted as positive
- Recall (sensitivity): success rate in the positive class (of the total positives, how many were detected)
- F1:. Harmonic average of precision and recall with the aim of giving a unique measure that equally values the mistakes made in either direction (FP or FN)
    - F1 = 2 x Precision x Recall/(Precision + Recall)

In [160…

```
# confusion matrix in sklearn

from sklearn.metrics import ConfusionMatrixDisplay, accuracy_score
from sklearn.metrics import confusion_matrix
from sklearn.metrics import classification_report

def matriz_confusao(actual, predicted):

    # outcome values order in sklearn
    matrix = confusion_matrix(y_true = actual, y_pred = predicted, labels=[True,
    disp = ConfusionMatrixDisplay(confusion_matrix=matrix, display_labels=[True,
    disp.plot()

    # classification report for precision, recall f1-score and accuracy
    matrix = classification_report(actual,predicted)
    print('Classification report : \n',matrix)

# chamada à função
res = matriz_confusao(y_test,ypred)
```

```
Classification report :
              precision    recall  f1-score   support

           0       0.96      0.98      0.97       103
           1       0.97      0.94      0.96        68

    accuracy                           0.96       171
   macro avg       0.97      0.96      0.96       171
weighted avg       0.97      0.96      0.96       171
```



e) Holdout - 10x

In [161…

```
# Holdout
#from sklearn.metrics import accuracy_score

# Initialize your machine learning model

model = DecisionTreeClassifier()

scores = []

# Iterate through each fold
for i in range(10):
    X_train,X_test,y_train,y_test=train_test_split(X,y,test_size=0.3)

    # Train the model on the training data
    clf.fit(X_train, y_train)

    # Make predictions on the test data
    y_pred = clf.predict(X_test)

    # Calculate the accuracy score for this fold
    fold_score = accuracy_score(y_test, y_pred)

    # Append the fold score to the list of scores
    scores.append(fold_score)

# Calculate the mean accuracy across all folds
mean_accuracy = np.mean(scores)
print("Holdout Scores:", scores)
print("Mean Accuracy:", mean_accuracy)
```

```
Holdout Scores: [0.9181286549707602, 0.9239766081871345, 0.9298245614035088, 0.9
064327485380117, 0.9064327485380117, 0.9181286549707602, 0.9532163742690059, 0.9
298245614035088, 0.9122807017543859, 0.9122807017543859]
Mean Accuracy: 0.9210526315789472
```

g) K-fold cross validation

In [162…

```
# K-Fold Cross Validation - implementation
#
# Splitting the Data into Folds

def kfold_indices(data, k):
    fold_size = len(data) // k
    indices = np.arange(len(data))
    folds = []
    for i in range(k):
        test_indices = indices[i * fold_size : (i + 1) * fold_size]
        train_indices = np.concatenate([indices[:i * fold_size], indices[(i + 1)
        folds.append((train_indices, test_indices))
    return folds

# Define the number of folds (K)
k = 5

# Get the fold indices
fold_indices = kfold_indices(X, k)
```

In [163…

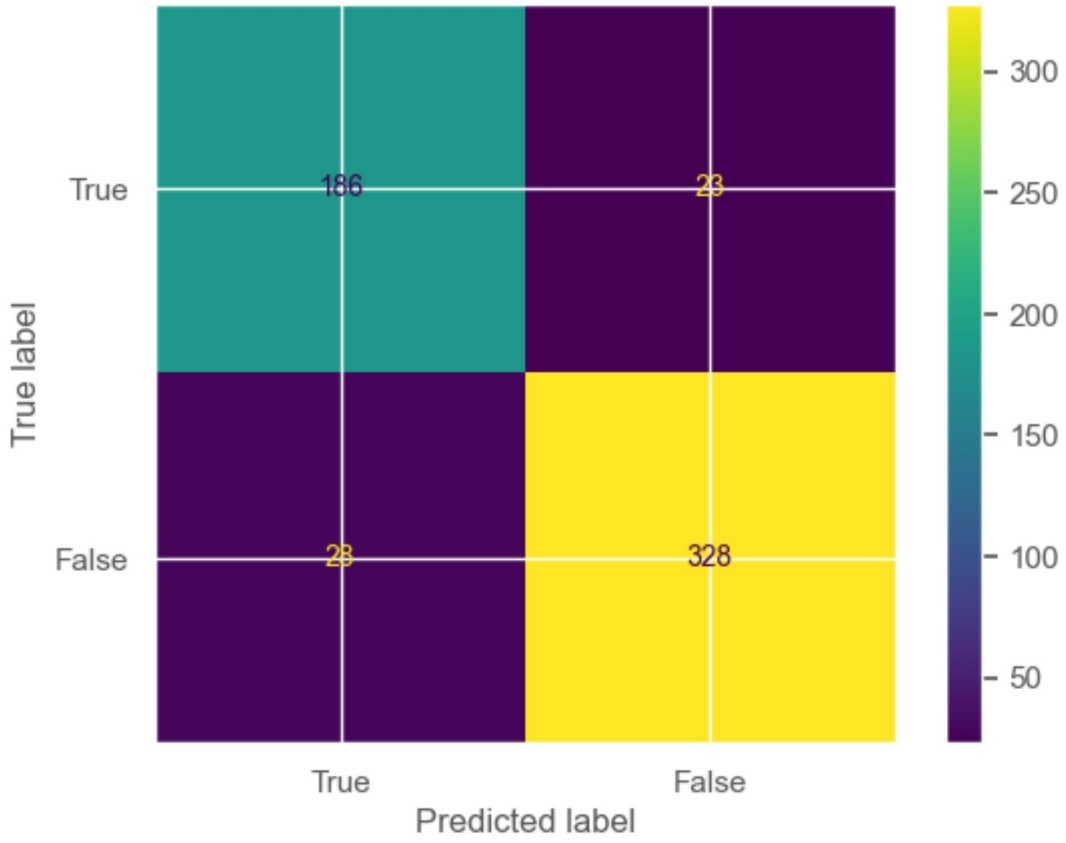
```python
# Performing K-Fold Cross-Validation
#from sklearn.metrics import accuracy_score

# Initialize your machine learning model

model = DecisionTreeClassifier()

scores = []
prevs_folds=[]
y_folds=[]
# Iterate through each fold
for train_indices, test_indices in fold_indices:
    X_train, y_train = X[train_indices], y[train_indices]
    X_test, y_test = X[test_indices], y[test_indices]

    # Train the model on the training data
    clf.fit(X_train, y_train)

    # Make predictions on the test data
    y_pred = clf.predict(X_test)

    # Calculate the accuracy score for this fold
    fold_score = accuracy_score(y_test, y_pred)

    # Append the fold score to the list of scores
    scores.append(fold_score)


    # Append the prevs and labels of the test set
    prevs_folds.append(y_pred)
    y_folds.append(y_test)


# Calculate the mean accuracy across all folds
mean_accuracy = np.mean(scores)
std_accuracy=np.std(scores)
print("K-Fold Cross-Validation Scores:", scores)
print("Mean Accuracy:", mean_accuracy)
print("Standart Deviation:", std_accuracy)
```

```
K-Fold Cross-Validation Scores: [0.8672566371681416, 0.9203539823008849, 0.95575
22123893806, 0.9557522123893806, 0.8495575221238938]
Mean Accuracy: 0.9097345132743364
Standart Deviation: 0.04421237520990018
```

In [164…

```python
resultados = matriz_confusao(np.concatenate(y_folds), np.concatenate(prevs_folds
```

```
Classification report :
              precision    recall  f1-score   support

           0       0.93      0.92      0.93       356
           1       0.87      0.89      0.88       209

    accuracy                           0.91       565
   macro avg       0.90      0.91      0.90       565
weighted avg       0.91      0.91      0.91       565
```



Hyperparameter tuning / Overfitting

In [165…

```
# The score on the training set is 100%, but the score on the test set is 95%. T
# Note that the decision tree model learned the training set very well, but the
# To overcome the overfitting problem, we control the complexity of a tree. We c
# which controls the maximum number of levels. The default value for the max_dep
# We can try a smaller value and compare the results. Let me specify the max_dep
```

In [166…

```
# Now we want to do some model exploration. For example, we mentioned above that
# If we wanted to study this dependency more systematically, we could repeat bui

X_train,X_test,y_train,y_test=train_test_split(X,y,test_size=0.3,random_state=12

import numpy as np
max_depths = np.array([1, 2, 3, 4, 5, 6, 7, 8, 9, 10])
```

In [167…

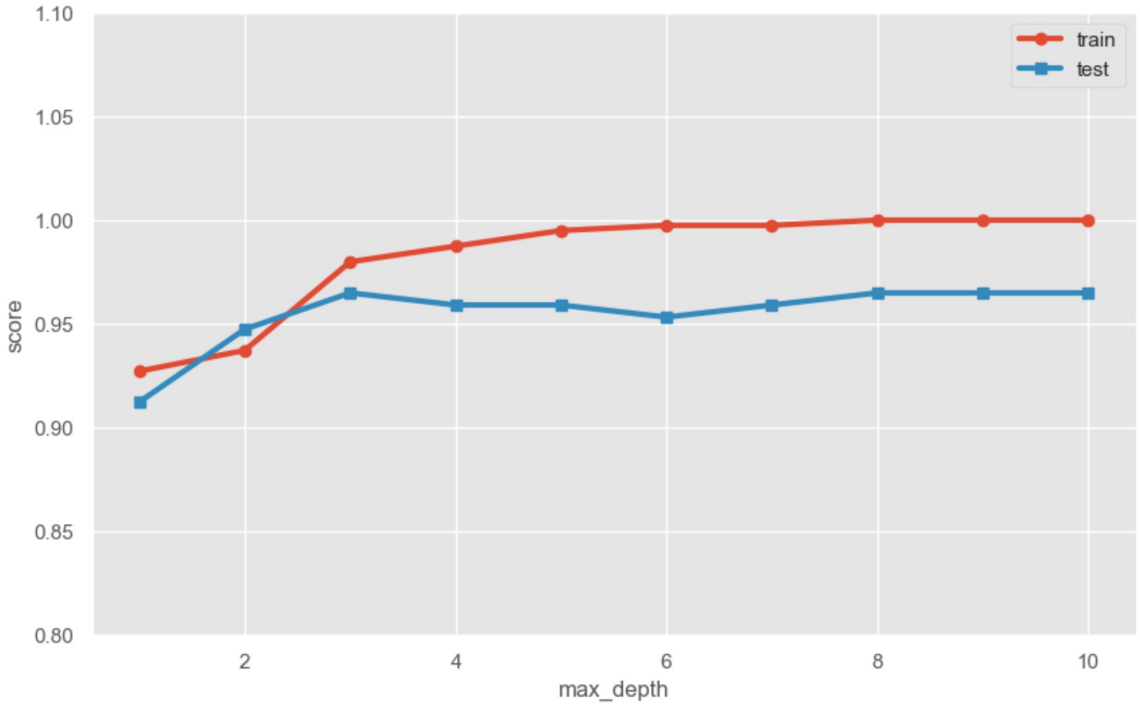
```
# For each of these values, we want to run the full model cascade from start to
# We also want to record the train and test scores. We do this in a for loop:

train_score = []
test_score = []
for d in max_depths:
    clf = DecisionTreeClassifier(max_depth=d, random_state=42)
    clf.fit(X_train, y_train)
    train_score.append(clf.score(X_train, y_train))
    test_score.append(clf.score(X_test, y_test))
```

In [168…

```
# We can plot the scores as a function of the tree depth using Matplotlib:

import matplotlib.pyplot as plt

%matplotlib inline
plt.style.use('ggplot')
```

In [169…

```
plt.figure(figsize=(10, 6))
plt.plot(max_depths, train_score, 'o-', linewidth=3, label='train')
plt.plot(max_depths, test_score, 's-', linewidth=3, label='test')
plt.xlabel('max_depth')
plt.ylabel('score')
plt.ylim(0.8, 1.1)
plt.legend();
```



In [170…

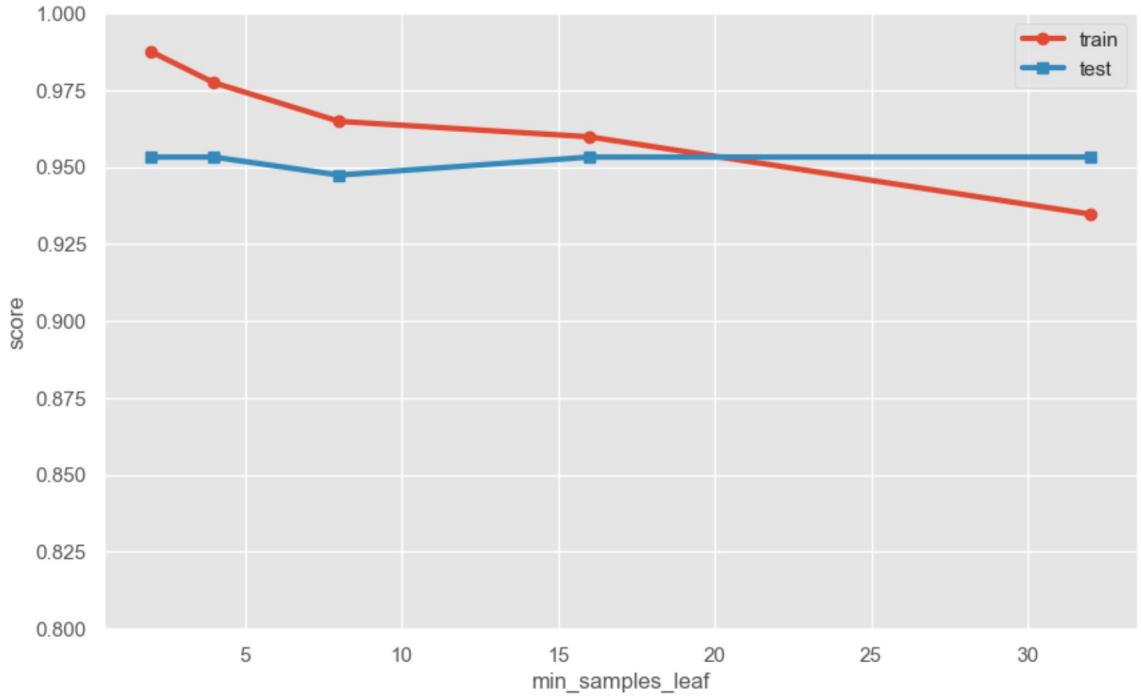
```
# What about the minimum numbers of samples required to make a node a leaf node?

train_score = []
test_score = []
min_samples = np.array([2, 4, 8, 16, 32])
for s in min_samples:
    clf = DecisionTreeClassifier(min_samples_leaf=s, random_state=42)
    clf.fit(X_train, y_train)
    train_score.append(clf.score(X_train, y_train))
    test_score.append(clf.score(X_test, y_test))
```

In [171…

```
plt.figure(figsize=(10, 6))
plt.plot(min_samples, train_score, 'o-', linewidth=3, label='train')
plt.plot(min_samples, test_score, 's-', linewidth=3, label='test')
plt.xlabel('min_samples_leaf')
plt.ylabel('score')
plt.ylim(0.8, 1)
plt.legend()
```

Out[171]:

```
<matplotlib.legend.Legend at 0x20b00411750>
```



Hint: To find the best parameters, we can use GridSearchCV #(https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.GridSearchCV.html) # Refs: # https://tirendazacademy.medium.com/breast-cancer-detection-with-decision-trees-f66637ac482e # https://www.kaggle.com/code/nisasoylu/decision-tree-implementation-on-cancer-dataset?scriptVersionId=38312678&cellId=28 # https://scikit-learn.org/stable/auto_examples/tree/plot_unveil_tree_structure.html#sphx-glr-auto-examples-tree-plot-unveil-tree-structure-py

In [ ]: