Investigations of Supervised Machine Learning Algorithm: Classification

This project explores various supervised machine learning algorithms and evaluate their performance scores. This proejct focuses on classification, analyzing pros and cons and determing when to use each of them.

This project works with the Breast Cancer Wisconsin dataset. Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image.

For more information, see https://archive.ics.uci.edu/ml/datasets/breast+cancer+wisconsin+(diagnostic)

Table of Contents

- Train an artifical neural network using `MLPClassifier`

Part 4: Neural Network

- Define and train a simple Neural-Network with `PyTorch` and use it via `skorch` with `SciKit-Learn`. Bulid ANN.

PART 0: Understanding the data

In [220…
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.datasets import load_breast_cancer
```

In [221…
```
cancer = load_breast_cancer()

df = pd.DataFrame(data=cancer.data, columns=cancer.feature_names)
df.head()
```

Out[221]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	dim
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	0.2419	0
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	0.1812	0
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	0.2069	0
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	0.2597	0
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	0.1809	0

5 rows × 30 columns

In [222…
```
df.describe()
```

Out[222]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean con p
count	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.00
mean	14.127292	19.289649	91.969033	654.889104	0.096360	0.104341	0.088799	0.04
std	3.524049	4.301036	24.298981	351.914129	0.014064	0.052813	0.079720	0.03
min	6.981000	9.710000	43.790000	143.500000	0.052630	0.019380	0.000000	0.00
25%	11.700000	16.170000	75.170000	420.300000	0.086370	0.064920	0.029560	0.02
50%	13.370000	18.840000	86.240000	551.100000	0.095870	0.092630	0.061540	0.03
75%	15.780000	21.800000	104.100000	782.700000	0.105300	0.130400	0.130700	0.07
max	28.110000	39.280000	188.500000	2501.000000	0.163400	0.345400	0.426800	0.20

8 rows × 30 columns

a. Total Sample Number, Feature Count/data type, Imblances/NA sample (If applicable)

In [223…

```
print('Sample number:', df.shape[0])
print('Feature count:', df.shape[1], "\n")

print("Number of NaN values:", df.isna().sum().sum(), "\n")
print("Checking possible imbalances in classes:")
print(cancer['target_names'][0], np.count_nonzero(cancer['target'] == 0))
print(cancer['target_names'][1], np.count_nonzero(cancer['target'] == 1), "\n")
```

```
Sample number: 569
Feature count: 30

Number of NaN values: 0

Checking possible imbalances in classes:
malignant 212
benign 357
```

In [224…

```
print("Feature data types:")
print(df.dtypes)
print()
```

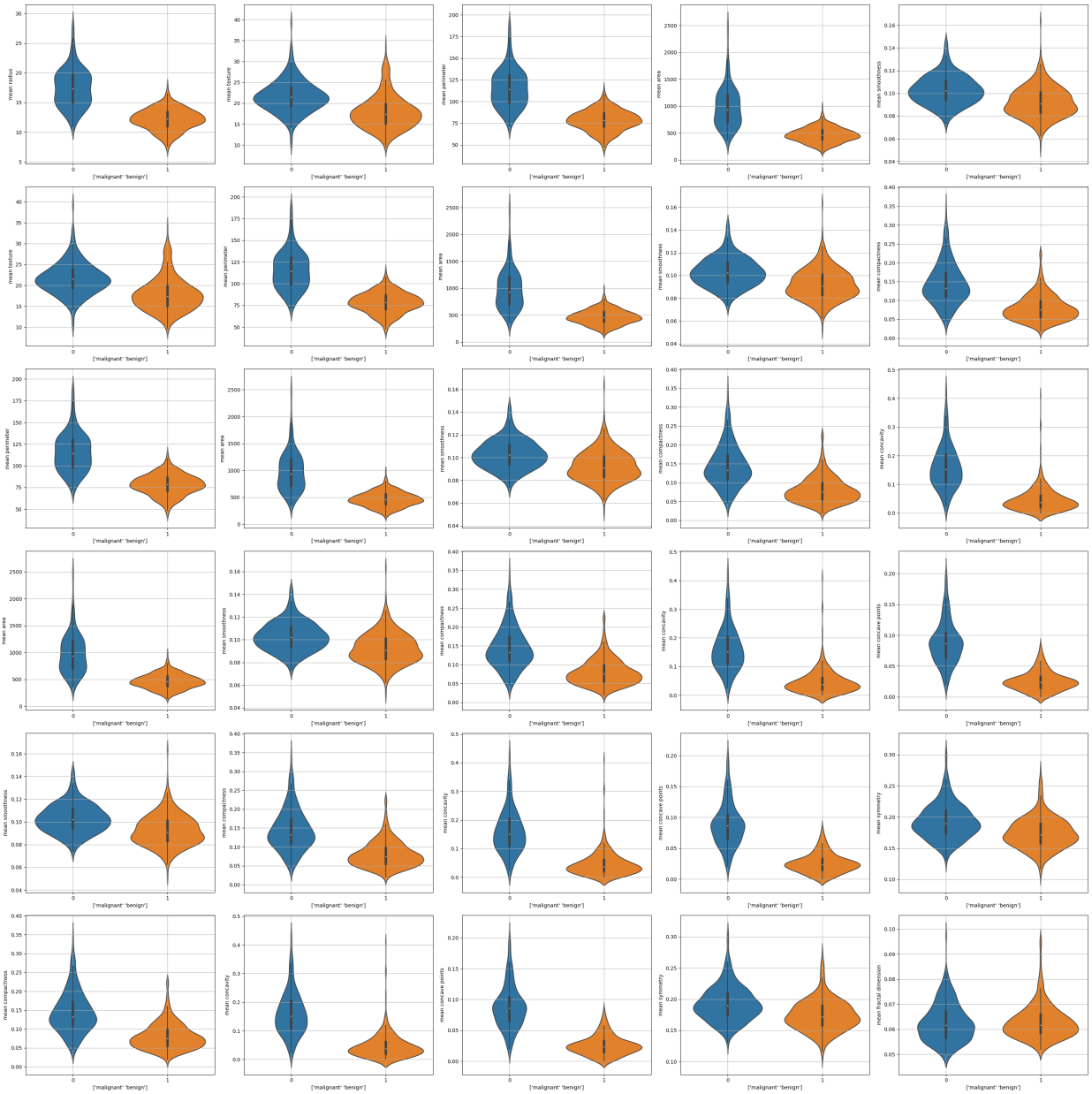
```
Feature data types:
mean radius                float64
mean texture               float64
mean perimeter             float64
mean area                  float64
mean smoothness            float64
mean compactness           float64
mean concavity             float64
mean concave points        float64
mean symmetry              float64
mean fractal dimension     float64
radius error               float64
texture error              float64
perimeter error            float64
area error                 float64
smoothness error           float64
compactness error          float64
concavity error            float64
concave points error       float64
symmetry error             float64
fractal dimension error    float64
worst radius               float64
worst texture              float64
worst perimeter            float64
worst area                 float64
worst smoothness           float64
worst compactness          float64
worst concavity            float64
worst concave points       float64
worst symmetry             float64
worst fractal dimension    float64
dtype: object
```

b. Distribution of the first four features using `violinplot`

Note that features are distributed in a wide range; minimum range:0.00-0.02 maximum range: 0-2500

In [225…

```
fig, axes = plt.subplots(6,5, figsize=(30,30))

for i in range(6):
    for j in range(5):
        sns.violinplot(ax=axes[i][j], x=cancer['target'], y=df.iloc[:,i+j])
        axes[i][j].set_xlabel(str(cancer['target_names']))
        axes[i][j].grid()
plt.tight_layout()
```

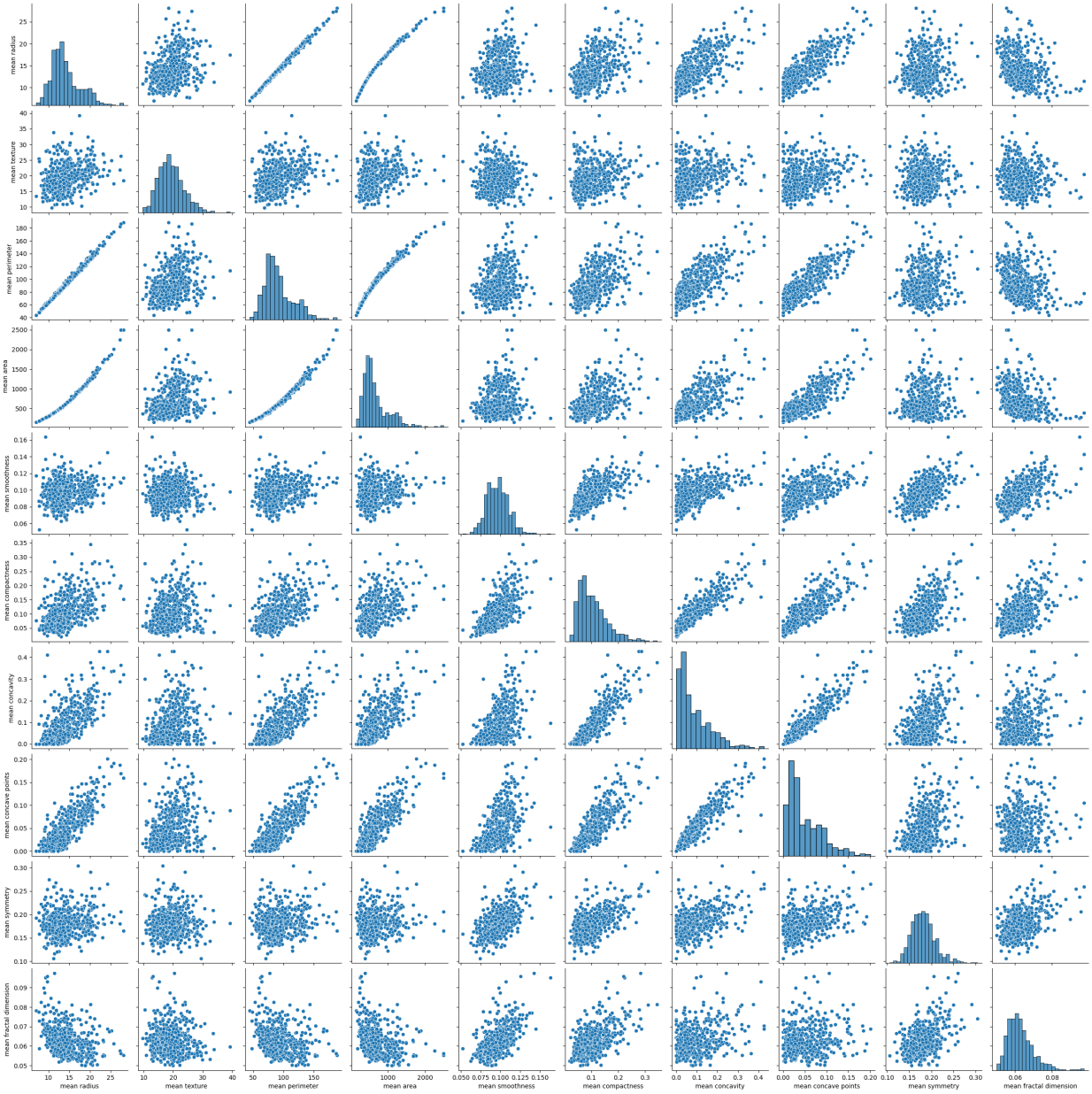


c. Distribution of features can be explored using `pairplot`.

I explored the first 10 features related to 'mean' for simplicity. The diagonal plots are univariate distribution plots, displaying the marginal distribution of the data in each column. Some features are shown to be highly linearly correlated, while others don't. In particular, mean texture and mean radius are linearly correlated, as well as mean area and mean perimeter are correlated in a linear/polynomial fashion. On the other hand, mean fractor and mean concave points do not show a clear relatinoship. One can conclude that there is no correlation between them, but consider that distribution of perimeter ranges from 50-200 while that of concave points ranges from 0-.2, adjusting values could solve the problem.

In [7]:
```
sns.pairplot(df.iloc[:,0:10])
```

Out[7]:
```
<seaborn.axisgrid.PairGrid at 0x2a6ee48e7f0>
```



d. Cleaning/Solving Imbalances of Data

The data is splitted into a training and validation set, at a ratio of 70/30. In order to reduce of sampling error in each set, the distribution of two classes are computed for both training and validation sets. Note that the relative percentages of each classes in each sets: there exists a slight difference in how data sets are split -- `stratify` enables splitting datasets into train/test sets *in terms of classes*.

In [226…

```
from sklearn.model_selection import train_test_split
from collections import Counter
X = cancer['data']
y = cancer['target']
print("Original Data (Pos/neg)")
print(cancer['target_names'][0], 0, np.count_nonzero(cancer['target'] == 0))
print(cancer['target_names'][1], 1, np.count_nonzero(cancer['target'] == 1), end="\n\r

# Part II 1-a&b
print("Before stratifying:")
```

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=.3, random_state=1
print(Counter(y_train))
print(Counter(y_test))
print("Relative percentage of training set: malignant = {:.5f}, benign = {:.5f}, combi
    Counter(y_train)[0]/np.count_nonzero(cancer['target'] == 0),
    Counter(y_train)[1]/np.count_nonzero(cancer['target'] == 1),
    ((Counter(y_train)[0]+Counter(y_train)[1]))/df.shape[0]))
print("Relative percentage of testing set: malignant = {:.5f}, benign = {:.5f}, combir
    Counter(y_test)[0]/np.count_nonzero(cancer['target'] == 0),
    Counter(y_test)[1]/np.count_nonzero(cancer['target'] == 1),
    (Counter(y_test)[0]+Counter(y_test)[1])/df.shape[0]))

print()

print("After stratifying:")
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=.3, stratify=y, ra
print(Counter(y_train))
print(Counter(y_test))

print("Relative percentage of training set: malignant = {:.5f}, benign = {:.5f}, combi
    Counter(y_train)[0]/np.count_nonzero(cancer['target'] == 0),
    Counter(y_train)[1]/np.count_nonzero(cancer['target'] == 1),
    (Counter(y_train)[0]+Counter(y_train)[1])/df.shape[0]))
print("Relative percentage of testing set: malignant = {:.5f}, benign = {:.5f}, combir
    Counter(y_test)[0]/np.count_nonzero(cancer['target'] == 0),
    Counter(y_test)[1]/np.count_nonzero(cancer['target'] == 1),
    (Counter(y_test)[0]+Counter(y_test)[1])/df.shape[0]))
```

```
Original Data (Pos/neg)
malignant 0 212
benign 1 357

Before stratifying:
Counter({1: 249, 0: 149})
Counter({1: 108, 0: 63})
Relative percentage of training set: malignant = 0.70283, benign = 0.69748, combined
= 0.69947
Relative percentage of testing set: malignant = 0.29717, benign = 0.30252, combined =
0.30053

After stratifying:
Counter({1: 250, 0: 148})
Counter({1: 107, 0: 64})
Relative percentage of training set: malignant = 0.69811, benign = 0.70028, combined
= 0.69947
Relative percentage of testing set: malignant = 0.30189, benign = 0.29972, combined =
0.30053
```

Part II: K-Nearest Neighbors

In [227…

```
from sklearn.neighbors import KNeighborsClassifier as knn
import warnings
warnings.filterwarnings('ignore')
```

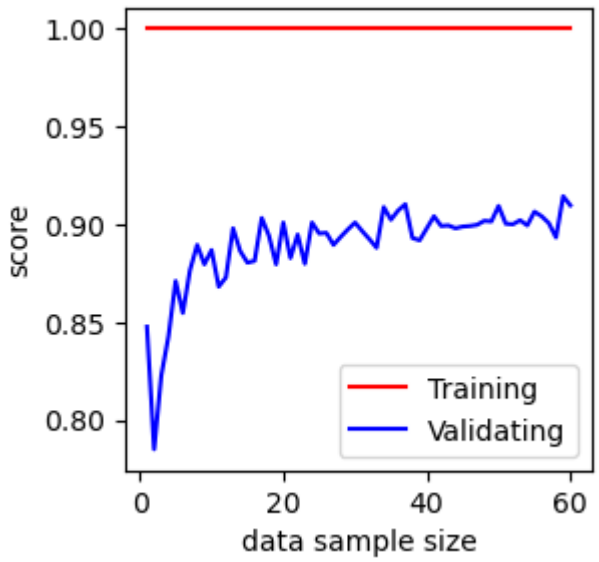
a-1. Exploring different k constants: setting k as 1

Setting k=1 results in training score to be 1, meaning the model is fitted based on single-nearest neighbour of the training set. Therefore, since the model is not generalized but rather is

highly specific to this training set **(i.e.overfitting)**, the score of 1 in the training set happens.

In [229…

```
avg_train = []
avg_valid = []
valid_dict = {i:0 for i in range(1,66)}
train_dict = {i:0 for i in range(1,66)}

for j in range(20):
    x_lst = []
    y_lst = []
    for i in range(1,66):
        model = knn(1)
        # construct a training set and validation set.
        X_train, X_test, y_train, y_test = train_test_split(X, y, train_size = i, test
        model.fit(X_train, y_train)
        x_lst.append(i) # List for plotting
        y_lst.append(model.score(X_test, y_test))

        # Record its training accuracy and validation accuracy (To compute average for
        valid_dict[i] += model.score(X_test, y_test)
        train_dict[i] += model.score(X_train, y_train)

for key in range(6,66):
    avg_valid.append(valid_dict[key]/20)
    avg_train.append(train_dict[key]/20)

x_average = np.linspace(1,60, num=60).reshape(-1,1)
y_avg_train = np.array(avg_train).reshape(-1,1)
y_avg_valid = np.array(avg_valid).reshape(-1,1)

plt.figure(figsize=(3,3))
plt.plot(x_average, y_avg_train, 'r')
plt.plot(x_average, y_avg_valid, 'b')
plt.xlabel('data sample size')
plt.ylabel('score')
plt.legend(['Training', 'Validating'])
plt.show()
```



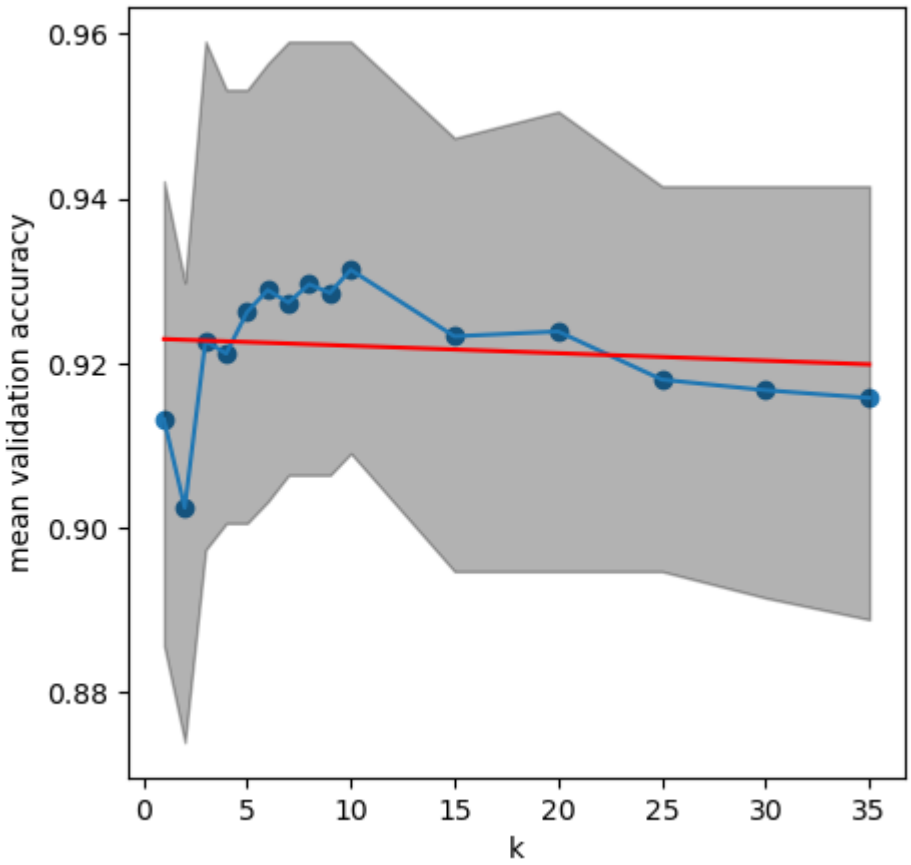
a-2. Exploring different k constants: deciding k hyperparameter

ean validation accuracy fluctuates when k is less than 10 (mean accuracy's behavior is not uniform when k is under 3, and the 90th percentile of the mean accuracy smoothens after k=10, as seen in the graph). Therefore, validation accuracy can be explained by a linear model after k=10. For this reason, I would choose k=10 since such k number has the highest stable accuracy.

In [233…

```
from sklearn.linear_model import LinearRegression
lst_k = [1,2,3,4,5,6,7,8,9,10,15,20,25,30,35]
result_dict = {}
for j in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X,y, stratify = y,test_size =
    result = []
    for i in lst_k:
        model1 = knn(i)
        model1.fit(X_train, y_train)
        result.append(model1.score(X_test, y_test))
    result_dict[j] = result

result_dict_rearranged = {i:[] for i in range(len(lst_k))}
for val in result_dict.values():
    for i in range(len(lst_k)):
        result_dict_rearranged[i].append(val[i])

avg_k = [sum(val)/50 for val in result_dict_rearranged.values()]

x2 = np.array(lst_k).reshape(-1,1)
y2 = np.array(avg_k).reshape(-1,1)
model2 = LinearRegression().fit(x2, y2)
y_pred = model2.predict(x2)
lin_eq = str(f"{model2.coef_}k + {model2.intercept_}")
print("y =", lin_eq)

plt.figure(figsize=(5,5))
plt.xlabel("k")
plt.ylabel("mean validation accuracy")
plt.scatter(lst_k, avg_k)
plt.plot(lst_k, avg_k)
plt.plot(x2, y_pred, color="red")

fifth = [np.percentile(v, 5) for v in result_dict_rearranged.values()]
nintyfifth = [np.percentile(v, 95) for v in result_dict_rearranged.values()]
plt.fill_between(lst_k, fifth, nintyfifth, color="k", alpha = .3)

plt.show()

print("Average score at k=10:", avg_k[9])
```

```
y = [[-9.04239766e-05]]k + [0.92302661]
```



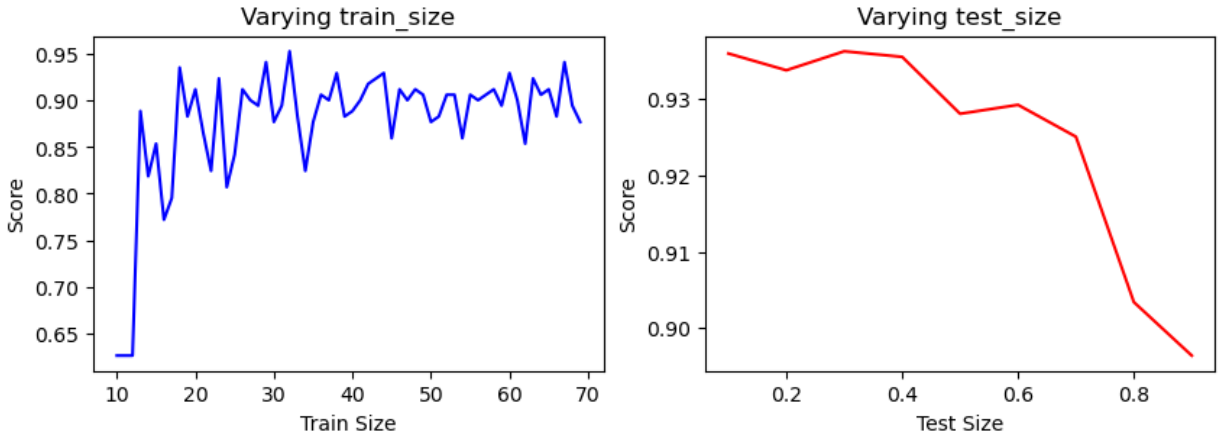

```
Average score at k=10: 0.9313450292397656
```

b.Exploring dependence on amounts of data

As seen in the blue graph, the larger dataset, the higher the knn model performs, but with a ceiling. Therefore, in order to increase the performance score, adding more data does not solve the problem. Whereas, the larger test size, the lower the model performs. Here, test_size=.3 is found to score the highest.

In [23]:
```
fig, axes = plt.subplots(1,2,figsize=(10,3))
x_lst = []
y_lst = []

# Fit a k-NN classifier with increasing amounts of data, from k to  60+k
for i in range(10,70):
    model = knn(10)
    X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, train_size =
    model.fit(X_train, y_train)
    x_lst.append(i)
    y_lst.append(model.score(X_test, y_test))

axes[0].plot( x_lst, y_lst, color="blue")
axes[0].set_xlabel('Train Size')
axes[0].set_ylabel('Score')
axes[0].set_title('Varying train_size')

# Fit a k-NN classifier with increasing test_size, ranges from 0.1 to 0.9
x_lst = np.linspace(0.1,0.9,9)
y_lst = [0]*9
for q in range(20):
```

```
    y_temp = []
    for j in np.linspace(0.1,.9,9):
        model = knn(10)
        X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_siz
        model.fit(X_train, y_train)
        y_temp.append(model.score(X_test, y_test)/20)
    y_lst = np.add(y_lst, y_temp)

plt.plot(x_lst, y_lst, color="r")
axes[1].set_xlabel('Test Size')
axes[1].set_ylabel('Score')
axes[1].set_title('Varying test_size')
plt.show()

#To see which test_size is score-optimal
plt.tight_layout()
print(x_lst)
print(y_lst)
```




```
[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9]
[0.93596491 0.93377193 0.93625731 0.93552632 0.92807018 0.92923977
 0.92506266 0.90339912 0.89639376]
<Figure size 640x480 with 0 Axes>
```

d. Adjust values using feature selection to increase performances

In [13]:
```
from sklearn.feature_selection import SequentialFeatureSelector
```

In [14]:
```
knn_model = knn(10).fit(X_train,y_train)
print(model.score(X_test, y_test))
```

```
0.9005847953216374
```

In [15]:
```
print(cancer.feature_names)
print(cancer.feature_names.shape)
```

```
['mean radius' 'mean texture' 'mean perimeter' 'mean area'
 'mean smoothness' 'mean compactness' 'mean concavity'
 'mean concave points' 'mean symmetry' 'mean fractal dimension'
 'radius error' 'texture error' 'perimeter error' 'area error'
 'smoothness error' 'compactness error' 'concavity error'
 'concave points error' 'symmetry error' 'fractal dimension error'
 'worst radius' 'worst texture' 'worst perimeter' 'worst area'
 'worst smoothness' 'worst compactness' 'worst concavity'
 'worst concave points' 'worst symmetry' 'worst fractal dimension']
(30,)
```

Using `SequentialFeatureSelector` from `sklearn`, features are chosen based on foward and backward selectors.

In [16]:
```
sfs_forward = SequentialFeatureSelector(
    knn_model, direction="forward"
).fit(X, y)

sfs_backward = SequentialFeatureSelector(
    knn_model, direction="backward"
).fit(X, y)
```

In [24]:
```
feature_names = cancer.feature_names
```

In [25]:
```
print("Forward Selection")
print(feature_names[sfs_forward.get_support()], "\n\tNumber of features:", feature_nam
print("Backward Selection")
print(print(feature_names[sfs_backward.get_support()], "\n\tNumber of features:", feat
```

```
Forward Selection
['mean smoothness' 'mean compactness' 'mean concavity'
 'mean concave points' 'mean fractal dimension' 'radius error'
 'smoothness error' 'compactness error' 'concavity error'
 'concave points error' 'symmetry error' 'fractal dimension error'
 'worst smoothness' 'worst concave points' 'worst fractal dimension']
       Number of features: 15

Backward Selection
['mean area' 'concavity error' 'concave points error' 'symmetry error'
 'fractal dimension error' 'worst radius' 'worst texture'
 'worst perimeter' 'worst area' 'worst smoothness' 'worst compactness'
 'worst concavity' 'worst concave points' 'worst symmetry'
 'worst fractal dimension']
       Number of features: 15

None
```

In [28]:
```
X_for = np.array(df.loc[:,feature_names[sfs_forward.get_support()]])
X_train, X_test, y_train, y_test = train_test_split(X_for,y,test_size = .3)

knn_for = knn(10).fit(X_train, y_train)
knn_for.score(X_test,y_test)
```

Out[28]:
```
0.935672514619883
```

In [29]:
```
X_back = np.array(df.loc[:,feature_names[sfs_backward.get_support()]])
X_train, X_test, y_train, y_test = train_test_split(X_back,y,test_size = .3)
```

```
knn_back = knn(10).fit(X_train, y_train)
knn_back.score(X_test,y_test)
```

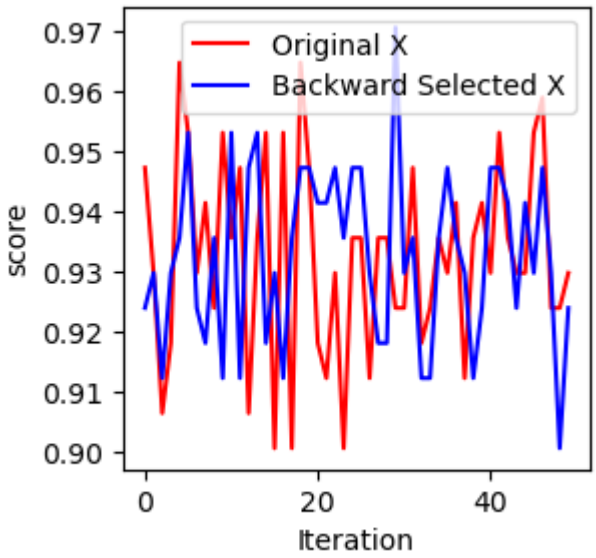
Out[29]:
```
0.9532163742690059
```

This has been done in order to prevent overfitting of datasets onto the model. Using knn model, it has been proven that backward selector results in a better score than forward selector does. Moreover, there is not much of a difference in the scores of the original and the backward datasets, even though the length of the original dataset is twice as big as the backward dataset. This clearly shows that overfitting happens in the original one.

However, features are selected based on knn model, it cannot be generalized that those selected features would prevent overfitting/improve performances for other models

In [30]:
```
X = cancer['data']
y = cancer['target']
```

In [33]:
```
score = []
score_back = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X,y,test_size = .3)
    knn_model = knn(10).fit(X_train, y_train)
    score.append(knn_model.score(X_test, y_test))

    X_train, X_test, y_train, y_test = train_test_split(X_back,y,test_size = .3)
    knn_model_back = knn(10).fit(X_train, y_train)
    score_back.append(knn_model_back.score(X_test, y_test))

plt.figure(figsize=(3,3))
plt.plot(score, 'r')
plt.plot(score_back, 'b')
plt.xlabel('Iteration')
plt.ylabel('score')
plt.legend(['Original X', 'Backward Selected X'])
plt.show()

print("Mean of the original X's score:", np.sum(score)/len(score))
print("Mean of the backward selection X's score:", np.sum(score_back)/len(score_back))
```




```
Mean of the original X's score: 0.9326315789473683
Mean of the backward selection X's score: 0.9327485380116957
```

Part III: Linear Regression Model

In [191…
```
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import RidgeCV
from sklearn.linear_model import Perceptron
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
```

Linear Regression model assumes that classes can be seperated based on a linear model. The basic form of linear regression model, y = b0+μ*b1, is influenced by variables b0 and b1. Note that they are heavily influenced on the *weights* of a data. This section experiments with such property, discussing how `normalize` changes the performance score of a linear regression model.

In [80]:
```
X = cancer['data']
y = cancer['target']
X_train, X_test, y_train, y_test = train_test_split(X,y,stratify=y,test_size = .3)
knn_model = knn(3)
knn_model.fit(X_train, y_train)

p_model = Perceptron(penalty='l2', alpha=1e-6, tol=1e-10)
p_model.fit(X_train, y_train)
```

Out[80]:
```
Perceptron(alpha=1e-06, penalty='l2', tol=1e-10)
```

`Confusion Matrix`, also known as an error matrix, is a specific table layout that allows visualization of the performance of an algorithm.

In [85]:
```
from sklearn import metrics

print("For knn: ")
print("Training score:", knn_model.score(X_train, y_train))
print("Testing score:", knn_model.score(X_test, y_test))
```

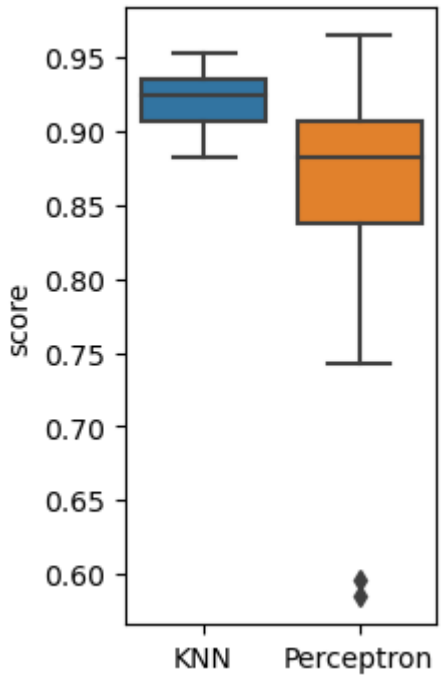
```
ypred1 = knn_model.predict(X_train)
print("confusion matrix")
print(metrics.confusion_matrix(y_train, ypred1))

print()

print("For perceptron: ")
print("Training score:", p_model.score(X_train, y_train))
print("Testing score:", p_model.score(X_test, y_test))
ypred2 = p_model.predict(X_train)
print("confusion matrix")
print(metrics.confusion_matrix(y_train, ypred2))
```

```
For knn:
Training score: 0.9623115577889447
Testing score: 0.9181286549707602
confusion matrix
[[138  10]
 [  5 245]]

For perceptron:
Training score: 0.7587939698492462
Testing score: 0.695906432748538
confusion matrix
[[ 52  96]
 [  0 250]]
```

Knn model seems to perform better, as the average score for knn is higher with small variance. Also, the interquartile range for perceptron is wider than that of knn, so in terms of precision, knn is also better.

In [87]:
```
knn_score = []
p_score = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3
    knn_model = knn(3)
    knn_model.fit(X_train, y_train)

    p_model = Perceptron(penalty='l2', alpha=1e-6, tol=1e-10)
    p_model.fit(X_train, y_train)

    knn_score.append(knn_model.score(X_test, y_test))
    p_score.append(p_model.score(X_test, y_test))

df_dict = {'KNN':knn_score, 'Perceptron':p_score}
df = pd.DataFrame(df_dict)

plt.figure(figsize=(2,4))
sns.boxplot(data=df)
plt.ylabel('score')
```

Out[87]:
```
Text(0, 0.5, 'score')
```

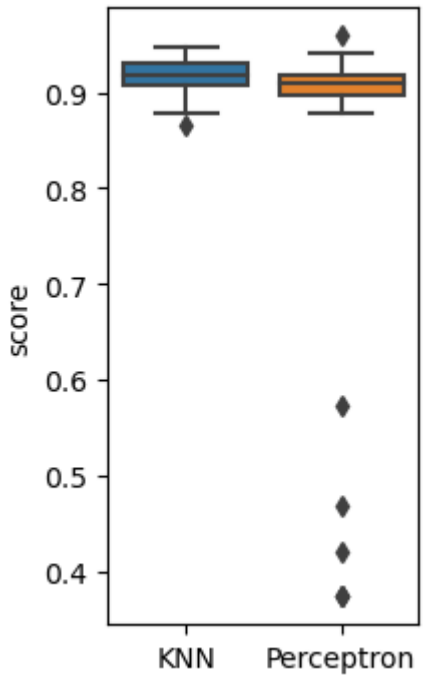


In [74]:
```
from sklearn.preprocessing import normalize
```

After normalization, the average score for knn remains the same, but that for perceptron increases alot. This may be because perceptron is heavily reliant on "weight". The data's features have different scales of measurements.This means that there are large input values, which can increase the weight of perceptron model, leading to higher generalization error. By normalizing the data, the weight is not overestimated, leading to the increase in perceptron score.

In [88]:
```
X_norm = normalize(X)

knn_score = []
p_score = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X_norm, y, stratify=y, test_si
    knn_model = knn(3)
    knn_model.fit(X_train, y_train)

    p_model = Perceptron(penalty='l2', alpha=1e-6, tol=1e-10)
    p_model.fit(X_train, y_train)

    knn_score.append(knn_model.score(X_test, y_test))
    p_score.append(p_model.score(X_test, y_test))

df_dict = {'KNN':knn_score, 'Perceptron':p_score}
df = pd.DataFrame(df_dict)

plt.figure(figsize=(2,4))
sns.boxplot(data=df)
plt.ylabel('score')
```

Out[88]:
```
Text(0, 0.5, 'score')
```

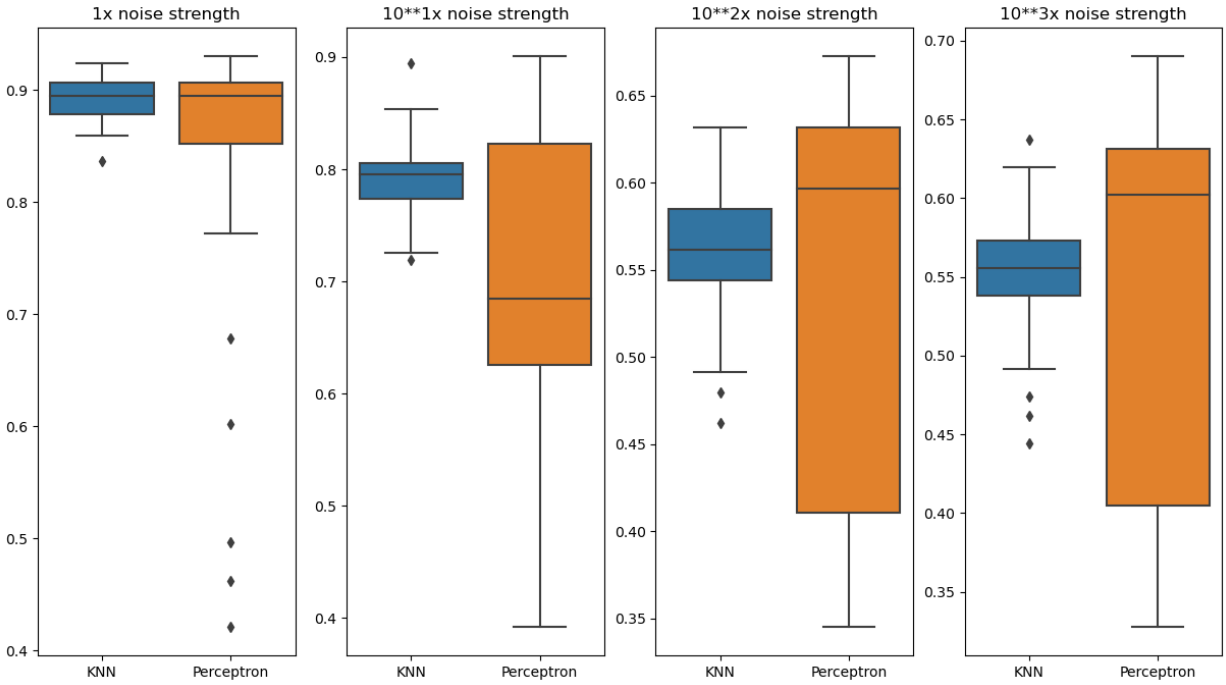


This section additionally experiments with the magnitude of data contamination on a model's performances by adding Gaussian noise to the features. I evaluated how the accuracy deteriorates for both algorihms as you increase the amount of contamination.

Gaussian noise with mean 0 and interquartile range of 4 different magnitudes is added -- 1, 10, 100, and 1000x. Accuracy of both knn and perceptron models decrease as the noise strength increases. Also, the interquartile range for the perceptron model increases more rapidly compared with knn. Interestingy, when the strength is set to be 1000, the interquartile ranges for both models increase, but the mean score also increases instead of decreasing.

In [89]:
```
fig, axes = plt.subplots(1,4, figsize = (15,8))

knn_score = []
p_score = []
for i in range(50):

    noise_strength = 1
    noise_col = np.transpose([noise_strength*np.random.rand(len(X_norm))])
    X_noise = np.concatenate((X_norm, noise_col), axis=1)

    X_train, X_test, y_train, y_test = train_test_split(X_noise, y, test_size=.3)
    knn_model = knn(3)
    knn_model.fit(X_train, y_train)

    p_model = Perceptron(penalty='l2', alpha=1e-6, tol=1e-10)
    p_model.fit(X_train, y_train)

    knn_score.append(knn_model.score(X_test, y_test))
    p_score.append(p_model.score(X_test, y_test))

df_dict = {'KNN':knn_score, 'Perceptron':p_score}
df = pd.DataFrame(df_dict)
sns.boxplot(ax=axes[0], data=df)
axes[0].set_title("1x noise strength")
```

```
for j in range(1,4):
    knn_score = []
    p_score = []
    for i in range(50):

        noise_strength = 10**j
        noise_col = np.transpose([noise_strength*np.random.rand(len(X_norm))])
        X_noise = np.concatenate((X_norm, noise_col), axis=1)

        X_train, X_test, y_train, y_test = train_test_split(X_noise, y, test_size=.3)
        knn_model = knn(3)
        knn_model.fit(X_train, y_train)

        p_model = Perceptron(penalty='l2', alpha=1e-6, tol=1e-10)
        p_model.fit(X_train, y_train)

        knn_score.append(knn_model.score(X_test, y_test))
        p_score.append(p_model.score(X_test, y_test))

    df_dict = {'KNN':knn_score, 'Perceptron':p_score}
    df = pd.DataFrame(df_dict)
    sns.boxplot(ax=axes[j], data=df)
    axes[j].set_title("10**{}x noise strength".format(j))
```



This section compares different linear regression model in terms of their score and predict vs. actual plots.

In [216…

```
lin_score = []
lin_pred = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X_norm, y, stratify=y, test_si
    lin_model = LinearRegression().fit(X_train,y_train)
    lin_score.append(lin_model.score(X_test, y_test))
    ypred = lin_model.predict(X_test)
    lin_pred.append([ypred, y_test])
```

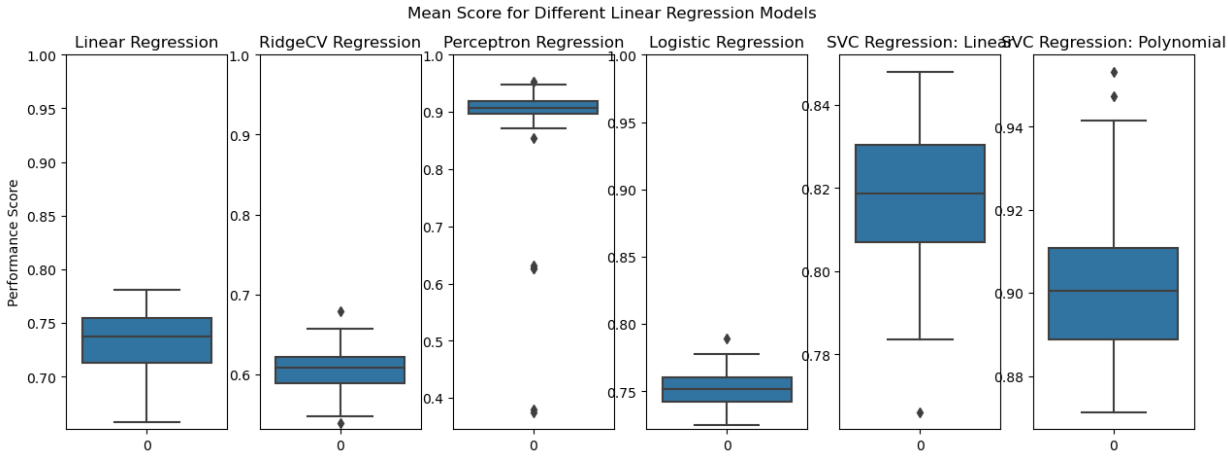
```
rcv_score = []
rcv_pred = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X_norm, y, stratify=y, test_si
    rcv_model = RidgeCV().fit(X_train,y_train)
    rcv_score.append(rcv_model.score(X_test, y_test))
    ypred = rcv_model.predict(X_test)
    rcv_pred.append([ypred, y_test])

perc_score = []
perc_pred = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X_norm, y, stratify=y, test_si
    perc_model = Perceptron().fit(X_train,y_train)
    perc_score.append(perc_model.score(X_test, y_test))
    ypred = perc_model.predict(X_test)
    perc_pred.append([ypred, y_test])

logreg_score = []
logreg_pred = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X_norm, y, stratify=y, test_si
    LogReg_model = LogisticRegression().fit(X_train,y_train)
    logreg_score.append(LogReg_model.score(X_test, y_test))
    ypred = LogReg_model.predict(X_test)
    logreg_pred.append([ypred, y_test])


svc_lin_score = []
svc_lin_pred = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X_norm, y, stratify=y, test_si
    svc_lin_model = SVC(kernel='linear').fit(X_train,y_train)
    svc_lin_score.append(svc_lin_model.score(X_test, y_test))
    ypred = svc_lin_model.predict(X_test)
    svc_lin_pred.append([ypred, y_test])

svc_poly_score = []
svc_poly_pred = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X_norm, y, stratify=y, test_si
    svc_poly_model = SVC(kernel='poly').fit(X_train,y_train)
    svc_poly_score.append(svc_poly_model.score(X_test, y_test))
    ypred = svc_poly_model.predict(X_test)
    svc_poly_pred.append([ypred, y_test])
```

In [217…

```
fig,axes = plt.subplots(1,6,figsize=(15,5))

sns.boxplot(ax=axes[0], data=lin_score)
sns.boxplot(ax=axes[1], data=rcv_score)
sns.boxplot(ax=axes[2], data=perc_score)
sns.boxplot(ax=axes[3], data=logreg_score)
sns.boxplot(ax=axes[4], data=svc_lin_score)
sns.boxplot(ax=axes[5], data=svc_poly_score)

axes[0].set_title("Linear Regression")
axes[1].set_title("RidgeCV Regression")
axes[2].set_title("Perceptron Regression")
axes[3].set_title("Logistic Regression")
```

```
axes[4].set_title("SVC Regression: Linear")
axes[5].set_title("SVC Regression: Polynomial")

for i in range(4):
    axes[i].set_ylim([None, 1])

axes[0].set_ylabel("Performance Score")
fig.suptitle("Mean Score for Different Linear Regression Models")
```

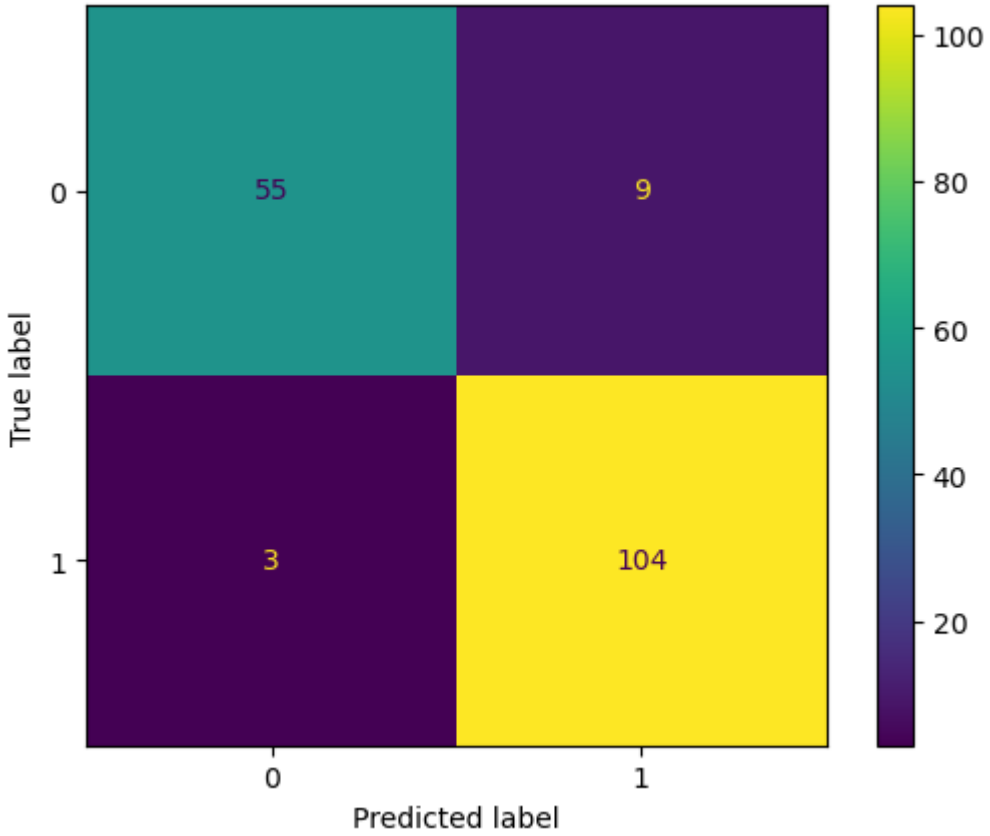
Out[217]:
```
Text(0.5, 0.98, 'Mean Score for Different Linear Regression Models')
```



Mean score for the perceptron model is found to be the highest. In-depth analysis on the perceptron is done using `metrics`. Note that while the score for successfully classifying data as benign is high, that for classifying as malignant is relatively low. Next section explores various *non-linear regressio models* to see if they can do better than the perceptron model.

In [218…
```
predict_test = perc_model.predict(X_test)
print("Average score:", np.sum(perc_score)/len(perc_score))
print("metrics accuracy", metrics.accuracy_score(y_test, ypred))
print("confusion matrix")
print(metrics.confusion_matrix(y_test,predict_test), "\n")

print(
    f"Classification report for classifier {perc_model}:\n"
    f"{metrics.classification_report(y_test, predict_test)}\n"
)

disp = metrics.ConfusionMatrixDisplay.from_predictions(y_test, predict_test)
```

```
Average score: 0.8719298245614034
metrics accuracy 0.9181286549707602
confusion matrix
[[ 55   9]
 [  3 104]]

Classification report for classifier Perceptron():
              precision    recall  f1-score   support

           0       0.95      0.86      0.90        64
           1       0.92      0.97      0.95       107

    accuracy                           0.93       171
   macro avg       0.93      0.92      0.92       171
weighted avg       0.93      0.93      0.93       171
```



Part IV: Non-linear Regression Model

SVC - rbf and sigmoid

`SVC` can be a non-linear model by changing its kernal type.

In [234…

```
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3)
svc_rbf_model = SVC(kernel='rbf').fit(X_train,y_train)
ypred = svc_rbf_model.predict(X_test)
print("metrics accuracy", metrics.accuracy_score(y_test, ypred))
print("confusion matrix")
print(metrics.confusion_matrix(y_test, ypred))
score = []
```

```
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3
    svc_rbf_model = SVC(kernel='rbf').fit(X_train,y_train)
    score.append(svc_rbf_model.score(X_test, y_test))

print("Average Score:", np.sum(score)/50)
```

```
metrics accuracy 0.9122807017543859
confusion matrix
[[ 49  15]
 [  0 107]]
Average Score: 0.911812865497076
```

In [235…

```
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3)
svc_sigmoid_model = SVC(kernel='sigmoid').fit(X_train,y_train)
ypred = svc_sigmoid_model.predict(X_test)
print("metrics accuracy", metrics.accuracy_score(y_test, ypred))
print("confusion matrix")
print(metrics.confusion_matrix(y_test, ypred))
score = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3
    svc_sigmoid_model = SVC(kernel='sigmoid').fit(X_train,y_train)
    score.append(svc_sigmoid_model.score(X_test, y_test))

print("Average Score:", np.sum(score)/50)
```

```
metrics accuracy 0.38011695906432746
confusion matrix
[[ 5 59]
 [47 60]]
Average Score: 0.4513450292397661
```

Tree Classifier

In [177…

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier
```

In [170…

```
X=cancer['data']
y=cancer['target']
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3)
```

In [171…

```
decision_model = DecisionTreeClassifier().fit(X_train, y_train)
ypred = decision_model.predict(X_test)
print("metrics accuracy", metrics.accuracy_score(y_test, ypred))
print("confusion matrix")
print(metrics.confusion_matrix(y_test, ypred))
```

```
metrics accuracy 0.9298245614035088
confusion matrix
[[60  4]
 [ 8 99]]
```

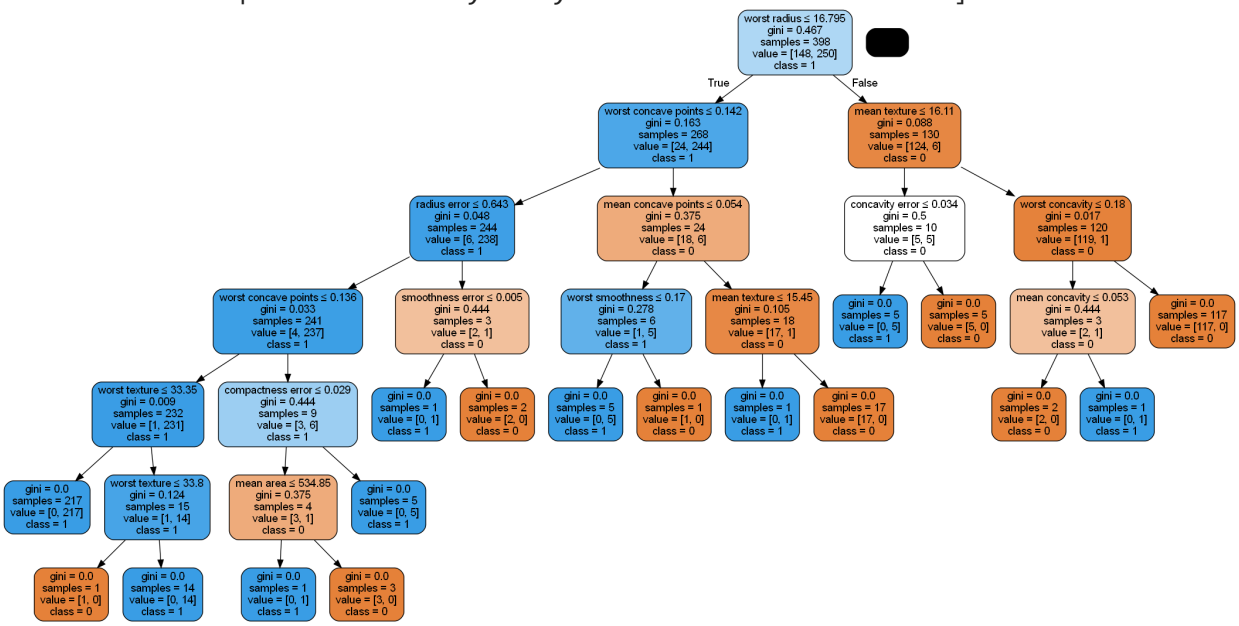
In [172…

```
import os
from sklearn.tree import export_graphviz
from six import StringIO
from IPython.display import Image
import pydotplus
dot_data = StringIO()
export_graphviz(decision_model, out_file=dot_data,
```

```
                filled=True, rounded=True,
                special_characters=True,feature_names = cancer.feature_names,class_nam
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
graph.write_png('liver-disease.png')
print(feature_names)

Image(graph.create_png())
```

```
['mean radius' 'mean texture' 'mean perimeter' 'mean area'
 'mean smoothness' 'mean compactness' 'mean concavity'
 'mean concave points' 'mean symmetry' 'mean fractal dimension'
 'radius error' 'texture error' 'perimeter error' 'area error'
 'smoothness error' 'compactness error' 'concavity error'
 'concave points error' 'symmetry error' 'fractal dimension error'
 'worst radius' 'worst texture' 'worst perimeter' 'worst area'
 'worst smoothness' 'worst compactness' 'worst concavity'
 'worst concave points' 'worst symmetry' 'worst fractal dimension']
```

Out[172]:



Decision tree classifier includes max_depth as its hyperparameter. This section examines which value of max_depth will lead to the highest performance score. The result shows that max_depth=4 results seems the best value in terms of performance score and elapsed time.

In [173…

```
import time
print("Depth\tPerformance Score\tElapsed Time")
print("-----\t-----------------\t------------")
for i in range(1,10):
    start_time = time.time()
    clf = DecisionTreeClassifier(max_depth = i).fit(X_train, y_train)
    end = time.time()
    print("{}\t{}\t{}".format(i, clf.score(X_test, y_test),end-start_time))
```

```
Depth   Performance Score       Elapsed Time
-----   -----------------       ------------
1       0.9181286549707602      0.004393339157104492
2       0.9239766081871345      0.0043790340423583984
3       0.9298245614035088      0.0032150745391845703
4       0.9415204678362573      0.002020597457885742
5       0.9239766081871345      0.00737452507019043
6       0.9239766081871345      0.008230447769165039
7       0.9415204678362573      0.011449813842773438
8       0.9298245614035088      0.008109807968139648
9       0.9239766081871345      0.010730743408203125
```

In [236…

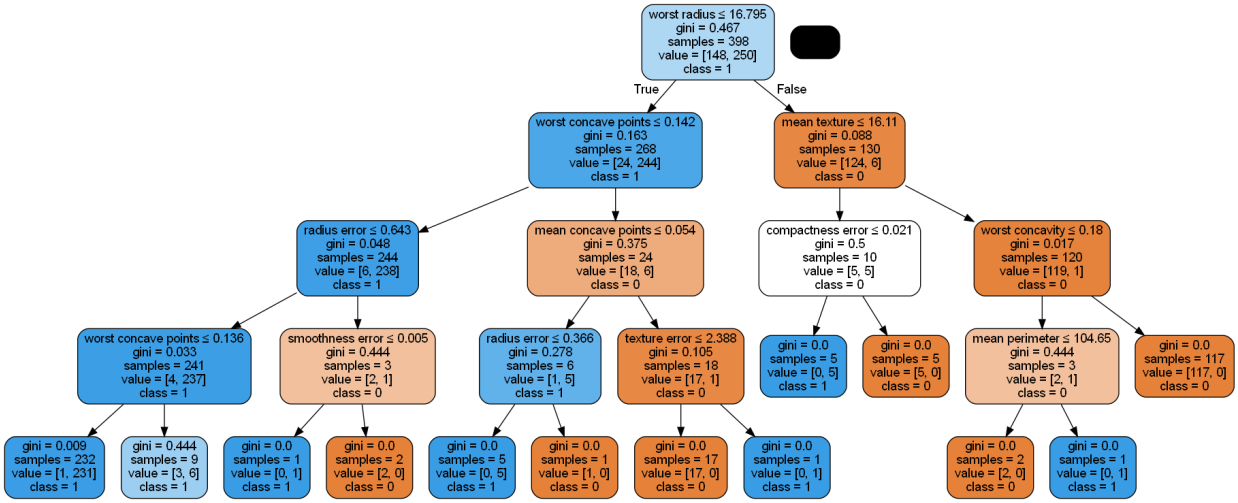
```
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3)
decision_model = DecisionTreeClassifier(max_depth=4).fit(X_train,y_train)
ypred = decision_model.predict(X_test)
print("metrics accuracy", metrics.accuracy_score(y_test, ypred))
print("confusion matrix")
print(metrics.confusion_matrix(y_test, ypred))
score = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3
    decision_model = DecisionTreeClassifier(max_depth=4).fit(X_train,y_train)
    score.append(decision_model.score(X_test, y_test))

print("Average Score:", np.sum(score)/50)
```

```
metrics accuracy 0.9239766081871345
confusion matrix
[[59  5]
 [ 8 99]]
Average Score: 0.9292397660818713
```

In [175…

```
import os
from sklearn.tree import export_graphviz
from six import StringIO
from IPython.display import Image
import pydotplus
dot_data = StringIO()
export_graphviz(decision_model, out_file=dot_data,
                filled=True, rounded=True,
                special_characters=True,feature_names = cancer.feature_names,class_nam
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
graph.write_png('liver-disease.png')

Image(graph.create_png())
```

Out[175]:



Testing `RandomForestClassifier` : It seems that performance score and elapsed time are not correlated with the number of depth. (The result shows that they are independent with each other). Setting max_depth = None, the score of random forest is found to be higher than than of decision tree.

In [180…

```
import time
print("Depth\tPerformance Score\tElapsed Time")
print("-----\t-----------------\t------------")
for i in range(1,20):
    start_time = time.time()
    clf = RandomForestClassifier(max_depth = i).fit(X_train, y_train)
    end = time.time()
    print("{}\t{}\t{}".format(i, clf.score(X_test, y_test),end-start_time))
```

```
Depth   Performance Score       Elapsed Time
-----   -----------------       ------------
1       0.9298245614035088      0.1889972686767578
2       0.9298245614035088      0.21786785125732422
3       0.9473684210526315      0.208831787109375
4       0.9532163742690059      0.20637845993041992
5       0.9532163742690059      0.2593259811401367
6       0.9473684210526315      0.2655951976776123
7       0.9532163742690059      0.2674868106842041
8       0.9532163742690059      0.24356985092163086
9       0.9532163742690059      0.2597970962524414
10      0.9532163742690059      0.25959229469299316
11      0.9532163742690059      0.24180126190185547
12      0.9532163742690059      0.2510993480682373
13      0.9590643274853801      0.25324058532714844
14      0.9590643274853801      0.24928712844848633
15      0.9473684210526315      0.2686185836791992
16      0.9532163742690059      0.30756044387817383
17      0.9532163742690059      0.25989770889282227
18      0.9532163742690059      0.27227163314819336
19      0.9473684210526315      0.25951361656188965
```

In [237…

```
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3)
rclf = RandomForestClassifier().fit(X_train,y_train)
ypred = rclf.predict(X_test)
print("metrics accuracy", metrics.accuracy_score(y_test, ypred))
print("confusion matrix")
print(metrics.confusion_matrix(y_test, ypred))
```

```
score = []
for i in range(50):
    X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, test_size=.3
    rclf = RandomForestClassifier().fit(X_train,y_train)
    score.append(rclf.score(X_test, y_test))

print("Average Score:", np.sum(score)/50)
```

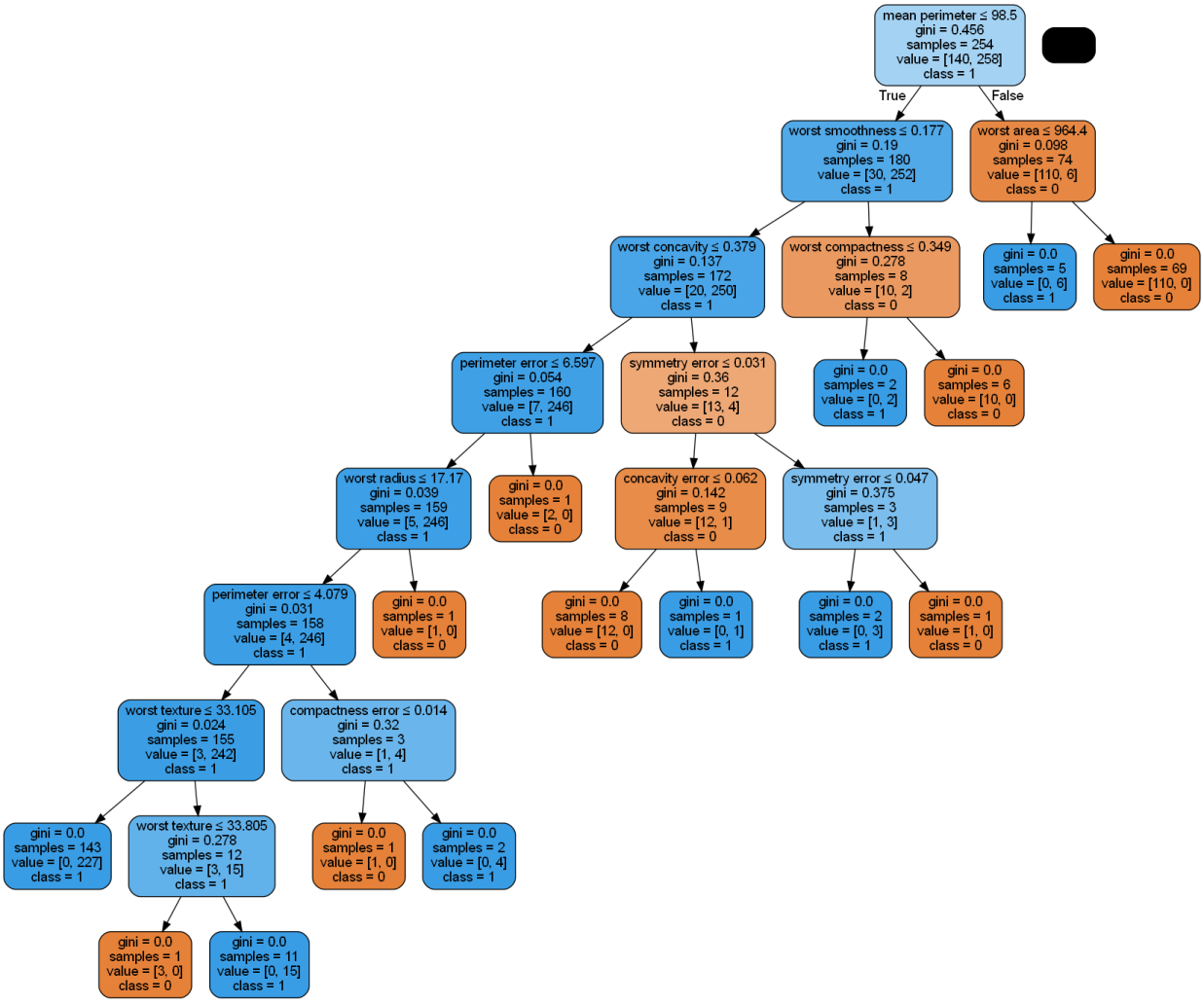
```
metrics accuracy 0.9649122807017544
confusion matrix
[[ 58   6]
 [  0 107]]
Average Score: 0.9581286549707602
```

This is the visualization of the first tree used in the random forest model.

In [183…

```
import os
from sklearn.tree import export_graphviz
from six import StringIO
from IPython.display import Image
import pydotplus
dot_data = StringIO()
export_graphviz(rclf.estimators_[0], out_file=dot_data,
                filled=True, rounded=True,
                special_characters=True,feature_names = cancer.feature_names,class_nam
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
graph.write_png('liver-disease.png')

Image(graph.create_png())
```

Out[183]:



Neural Network: ANN

MLPClassifier has lots of hyperparameters to choose from. For the simplicity, here, the number of hidden layer is set to be 1, since in general, one hidden layer is sufficient for the large majority of problems.

hidden_layer_sizes: The most commonly relied on is 'the optimal size of the hidden layer is usually between the size of the input and size of the output layers'. Reference: "Introduction to Neural Networks in Java" by Jeff Heaton. Therefore, the number of nodes is chosen to be the mean of input + output nodes.

activation: There are several options to choose: {identity', 'logistic', 'tanh', 'relu'}.

solver: {'lbfgs', 'sgd', 'adam'}, default='adam'

alpha: parameter to prevent overfitting. The higher the value is, more restriction is done to prevent overfitting.

In [456…

```
from sklearn.neural_network import MLPClassifier
mlp_model = MLPClassifier(hidden_layer_sizes=((df.shape[1]+2)//2), activation='relu',
print("score for training:", mlp_model.score(X_train, y_train))
print("score for testing:", mlp_model.score(X_test, y_test))
```

```
predict_test = mlp_model.predict(X_test)

print("metrics accuracy", metrics.accuracy_score(y_test, predict_test))
print("confusion matrix")
print(metrics.confusion_matrix(y_test, predict_test))
```

```
score for training: 0.8819095477386935
score for testing: 0.9298245614035088
metrics accuracy 0.9298245614035088
confusion matrix
[[ 56   7]
 [  5 103]]
```

Part V: Build Neural Network with PyTorch

Simple, fully connected neural network with one hidden layer. Input layer has 30 nodes, hidden layer has 100 and output layer 2 neurons.

In [457…
```
import torch
from torch import nn
import torch.nn.functional as F
```

In [458…
```
X = cancer.data.astype('float32')
y = cancer.target.astype('int64')
```

In [459…
```
device = 'cuda' if torch.cuda.is_available() else 'cpu'
```

In [460…
```
data_dim = X.shape[1]
hidden_dim = 1000
output_dim = len(np.unique(cancer.target))
data_dim, hidden_dim, output_dim
```

Out[460]:
```
(30, 1000, 2)
```

In [461…
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=
print(X_train.dtype)
```

```
float32
```

A Neural network in PyTorch's framework.

In [481…
```
class ClassifierModule(nn.Module):
    def __init__(
            self,
            input_dim=data_dim,
            hidden_dim=hidden_dim,
            output_dim=output_dim,
            dropout=.5, #Threshold to reduce noise
    ):
        super(ClassifierModule, self).__init__()
        self.dropout = nn.Dropout(dropout)

        self.hidden = nn.Linear(input_dim, hidden_dim)
        self.output = nn.Linear(hidden_dim, output_dim)

    def forward(self, X, **kwargs):
```

```
        X = F.relu(self.hidden(X)) #Use relu as its hidden layer's activation functior
        X = self.dropout(X)
        X = F.softmax(self.output(X), dim=-1)#Use softmax as its output layer's activa
        return X
```

In [477…
```
print(ClassifierModule())
```

```
ClassifierModule(
  (dropout): Dropout(p=1, inplace=False)
  (hidden): Linear(in_features=30, out_features=1000, bias=True)
  (output): Linear(in_features=1000, out_features=2, bias=True)
)
```

In [478…
```
from skorch import NeuralNetClassifier
```

In [479…
```
torch.manual_seed(0)

net = NeuralNetClassifier(
    ClassifierModule,
    max_epochs=20, #iteration number
    lr=0.1, #learning rate
    device=device,
)
```

In [480…
```
net.fit(X_train,y_train)
```

```
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6952       0.6250        5.9784  0.0445
      2        0.6861       0.6250        5.9784  0.0527
      3        0.6795       0.6250        5.9784  0.0500
      4        0.6746       0.6250        5.9784  0.0500
      5        0.6711       0.6250        5.9784  0.0420
      6        0.6684       0.6250        5.9784  0.0500
      7        0.6665       0.6250        5.9784  0.0499
      8        0.6651       0.6250        5.9784  0.0500
      9        0.6641       0.6250        5.9784  0.0505
     10        0.6633       0.6250        5.9784  0.0571
     11        0.6628       0.6250        5.9784  0.0488
     12        0.6624       0.6250        5.9784  0.0479
     13        0.6621       0.6250        5.9784  0.0555
     14        0.6618       0.6250        5.9784  0.0452
     15        0.6617       0.6250        5.9784  0.0467
     16        0.6616       0.6250        5.9784  0.0419
     17        0.6615       0.6250        5.9784  0.0481
     18        0.6614       0.6250        5.9784  0.0496
     19        0.6614       0.6250        5.9784  0.0507
     20        0.6614       0.6250        5.9784  0.0448
```

Out[480]:
```
<class 'skorch.classifier.NeuralNetClassifier'>[initialized](
  module_=ClassifierModule(
    (dropout): Dropout(p=1, inplace=False)
    (hidden): Linear(in_features=30, out_features=1000, bias=True)
    (output): Linear(in_features=1000, out_features=2, bias=True)
  ),
)
```

In [415…
```
y_pred = net.predict(X_test)
metrics.accuracy_score(y_test, y_pred)
```

Out[415]: 0.631578947368421