Homework 4

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Homework Description

- Course: ECEN649, Fall2022
- Deadline: 2022/11/16, 11:59 pm > Problems from the Book > > 6.3 > > 6.5 > > 6.7 > > 7.1 > > 7.10 > > 6.12 (coding assignment) > > Problems 6.3-6.5 are worth 10 points each, Problem 7.10 and the coding assignment are worth 20 points each.

Computational Environment

Libraries

```python
import numpy as np
import tensorflow as tf
import matplotlib.pyplot as plt
import sys
```

Versions

```python
print(np.__version__)
print(tf.__version__)
print (sys.version)
print(sys.executable)
```

```
1.23.4
2.10.0
3.9.12 (main, Apr  5 2022, 01:52:34)
[Clang 12.0.0 ]
/Users/stevenchiu/miniconda/bin/python
```

Problem 6.3

Show that the decision regions produced by a neural network with k threshold sigmoids in the *first* hidden layer, no matter what nonlinearities are used in succeeding layers, are equal to the intersection of k half-spaces, i.e., the decision boundary is piecewise linear

Hint: All neurons in the first hidden layer are perceptrons and the output of the layer is a binary vector.

Let $\bar{O}$ be the k output of first hidden layer, and there are 2^k types of binary vectors $[O_1, \dots, O_k]$.

For each data point $x \in R^d$ where d is the feature space. the output of first layer is

$$O(x)_i = I_{g_i(x)}(x), \quad i = 1, \cdots, k \tag{1}$$

where $g_i(\cdot)$ is the perceptron function of neuron i. Thus, any point x belong to one type of $[I_{g_1(x)}(x), \dots, I_{g_k(x)}(x)]$. For each O_i, the space forms a half-space with $\{x : g_i(x) > 0\}$, and there are k half space in total.

Problem 6.5

For the VGG16 CNN architecture:

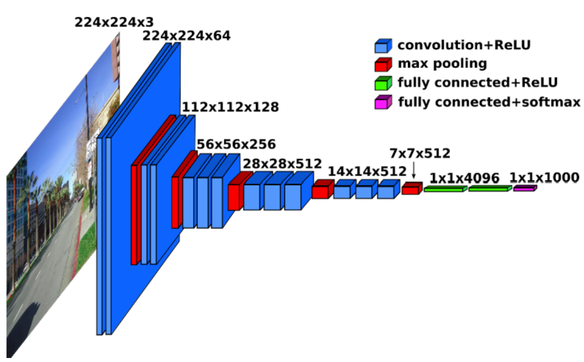


Figure 1: VGG16

(a)

Determine the number of filters used in each convolution layer.

- `Conv-1`: 64 filters (pre-depth: 3)
- `Conv-2`: 128 filters (pre-depth: 64)
- `Conv-3`: 256 filters (pre-depth: 128)
- `Conv-4`: 512 filters (pre-depth: 256)
- `Conv-5`: 512 filters (pre-depth: 512)

There are total

```
rs = np.array([3, 64, 128, 256, 512])
t_filters = np.array([64, 128, 256, 512, 512])
np.sum(t_filters)
```

```
1472
```

filters.

(b)

Based on the fact that all filters are of size $3 \times 3 \times r$, where r is the depth of the previous layer, determine the total number of convolution weights in the entire network.

```
CONV1 = (3*3*3)*64 + (3*3*64)*64
CONV1
```

```
38592
```

```
CONV2 = (3*3*64)*128 + (3*3*128)*128
CONV2
```

```
221184
```

```
CONV3 = (3*3*128)*256 + (3*3*256)*256 + (3*3*256)*256
CONV3
```

```
1474560
```

```
CONV4 = (3*3*256)*512 + (3*3*512)*512 + (3*3*512)*512
CONV4
```

```
5898240
```

```
CONV5 = (3*3*512)*512 *3
CONV5
```

```
7077888
```

```
fc1 = 512 * 7 * 7 * 4096
fc1
```

```
102760448
```

```
fc2 = 4096 * 4096
fc2
```

```
16777216
```

```
fc3 = 4096 * 1000
fc3
```

```
4096000
```

(c)

> Add the weights used in the fully-connected layers to obtain the total number of weights used by VGG16.

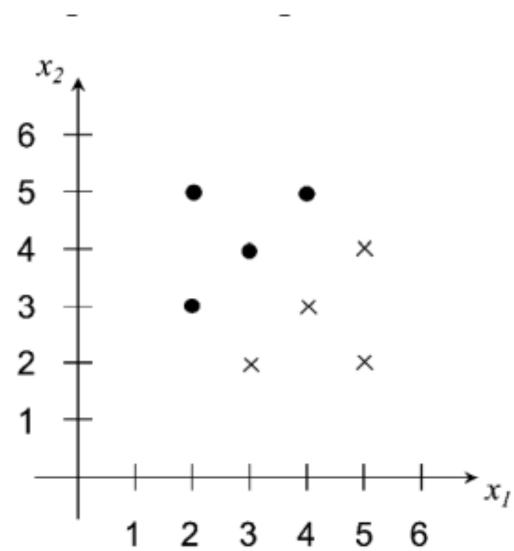
Total of weights

```
total = np.sum([CONV1, CONV2, CONV3, CONV4, CONV5, fc1, fc2, fc3])
total
```

```
138344128
```

Problem 6.7

Consider the training data set given in the figure below.



(a)

By inspection, find the coefficients of the linear SVM hyperplane $a_1x_1+a_2x_2+a_0 = 0$ and plot it. What is the value of the margin? Say as much as you can about the values of the Lagrange multipliers associated with each of the points.

The boundary passes by $\frac{1}{2}((3,3)+(3,2)) = (3,2.5)$ and $\frac{1}{2}((3,4)+(4,3)) = (3.5,3.5)$

- $a_1 = 2.5 - 3.5 = -1$
- $a_2 = 3.5 - 3 = 0.5$
- $a_0 = 3 \cdot 3.5 - 3.5 \cdot 2.5 = 1.75$
- The boundary is

$$-x_1 + 0.5x_2 + 1.75 = 0$$

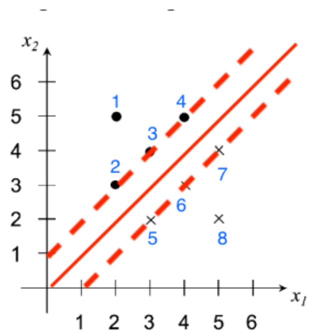


Figure 2: SVM boundry

In Figure 2, there are 6 support vectors that are λ_2 to λ_7. The KKT conditions[1] state that

$$\lambda_i = 0 \Rightarrow y_i E_i \leq 0 \tag{2}$$
$$0 < \lambda_i < C \Rightarrow y_i E_i = 0 \tag{3}$$
$$\lambda_i = C \Rightarrow y_i E_i \geq 0 \tag{4}$$

- Lagrange multipliers
  - $\lambda_1 = 0$
  - $\lambda_2 \in (0, C)$
  - $\lambda_3 \in (0, C)$
  - $\lambda_4 \in (0, C)$
  - $\lambda_5 \in (0, C)$
  - $\lambda_6 \in (0, C)$
  - $\lambda_7 \in (0, C)$
  - $\lambda_8 = 0$

where C is the pentalty term.

(b)

> Apply the CART rule, using the misclassification impurity, and stop after finding one splitting node (this is the "1R" or "stump" rule). If ther eis a tie between best splits, pick one that makes at most one error in each class. Plot this classifier as a decision boundary superimposed on the training data and also as a binary decision tree showing the splitting and leaf nodes.

where $\bullet$ labelled as 1; $\circ$ labelled as 0.

[1] Intro. to SVM: https://article.sciencepublishinggroup.com/html/10.11648.j.acm.s.2017060401.11.html

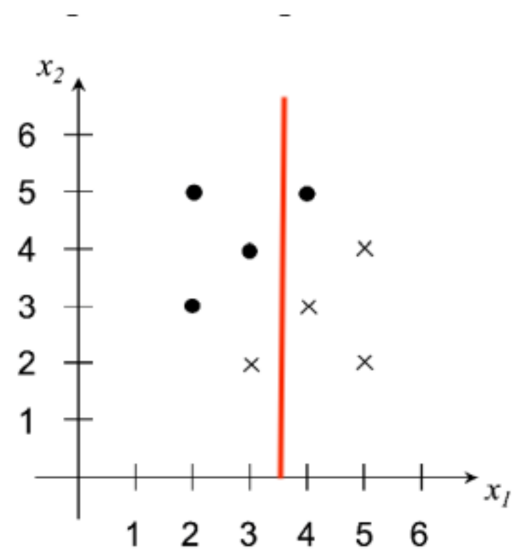


Figure 3: Decision boundary

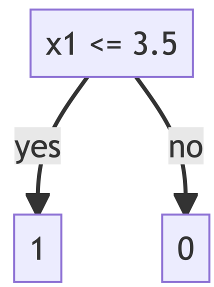


Figure 4: Apply CART rule

(c)

How do you compare the classifiers in (a) and (b) ? Which one is more likely to have a smaller classification error in this problem?

- SVM of (a) yields smaller classification error than (b) because it allow any slope of decision boundary.

Problem 7.1

Suppose that the classification error ϵ_n and an error estimator $\hat{\epsilon}_n$ are jointly Gaussian, such

$$\epsilon_n \sim N(\epsilon^* + \frac{1}{n}, \frac{1}{n^2}), \hat{\epsilon}_n \sim N(\epsilon^* - \frac{1}{n}, \frac{1}{n^2}), Cov(\epsilon_n, \hat{\epsilon}_n) = \frac{1}{2n^2}$$

where ϵ^* is the Bayes error. Find the bias, deviation variance, RMS, correlation coefficient and tail probabilities $P(\hat{\epsilon}_n - \epsilon_n < -\tau)$ and $P(\hat{\epsilon}_n - \epsilon_n > \tau)$ of $\hat{\epsilon}_n$. Is this estimator optimistically or pessimistically biased? Does performance improve as sample size increases? Is the estimator consistent?

Bias

Use Eq. 7.3 (Braga-Neto 2020, 154),

$$Bias(\hat{\epsilon}_n) = E[\hat{\epsilon}_n] - E[\epsilon_n]$$

- $E[\hat{\epsilon}_n] = \epsilon^* - \frac{1}{n}$
- $E[\epsilon_n] = \epsilon^* + \frac{1}{n}$

Thus,

$$Bias(\hat{\epsilon}_n) = \frac{-2}{n} < 0$$

This estimator is *optimisitcally biased*.

Deviation variance

Use Eq. 7.4 (Braga-Neto 2020, 154),

$$Var_{dev}(\hat{\epsilon}_n) = Var(\hat{\epsilon}_n, \epsilon_n) = Var(\hat{\epsilon}_n) + Var(\epsilon_n) - 2Cov(\epsilon_n, \hat{\epsilon}_n)$$

- $Var(\hat{\epsilon}_n) = \frac{1}{n^2}$
- $Var(\epsilon_n) = \frac{1}{n^2}$
- $Cov(\epsilon_n, \hat{\epsilon}_n) = \frac{1}{2n^2}$

Thus,

$$Var_{dev}(\hat{\epsilon}_n) = \frac{1}{n^2} + \frac{1}{n^2} - 2\frac{1}{2n^2} = \frac{1}{n^2}$$

The deviation variance reduces as sample size increases.

Root mean-square error

Use Eq. 7.5 (Braga-Neto 2020, 154),

$$RMS(\hat{\epsilon}_n) = \sqrt{E[(\hat{\epsilon}_n - \epsilon_n)^2]} = \sqrt{Bias(\hat{\epsilon}_n)^2 + Var_{dev}(\hat{\epsilon}_n)}$$

Apply previous results,

$$RMS(\hat{\epsilon}_n) = \sqrt{\frac{4}{n^2} + \frac{1}{n^2}} = \frac{\sqrt{5}}{n}$$

Correlation coefficient

Use the pearson correlation coefficient[2]

$$\rho_{X,Y} = \frac{Cov(X,Y)}{\sigma_X \sigma_Y}$$

- $Cov(\epsilon_n, \hat{\epsilon}_n) = \frac{1}{2n^2}$
- $\sigma_{\epsilon_n} = \frac{1}{n}$
- $\sigma_{\hat{\epsilon}_n} = \frac{1}{n}$

$$\rho_{\epsilon_n, \hat{\epsilon}_n} = \frac{1}{2}$$

Correlation coefficient is a constant and independent from sample size.

Tail probabilities

Use Eq. 7.6 (Braga-Neto 2020, 154),

$$P(|\hat{\epsilon}_n - \epsilon_n| \geq \tau) = P(\hat{\epsilon}_n - \epsilon_n \geq \tau) + P(\hat{\epsilon}_n - \epsilon_n \leq -\tau), \quad \text{for } \tau > 0$$

The normal difference distribution[3] of $\hat{\epsilon}_n - \epsilon_n$

$$\hat{\epsilon}_n - \epsilon_n \sim N(\frac{-2}{n}, \frac{2}{n^2}) = N(\mu, \sigma^2)$$

[2]Correlation coefficient: https://en.wikipedia.org/wiki/Pearson_correlation_coefficient
[3]Normal difference distribution: https://mathworld.wolfram.com/NormalDifferenceDistribution.html

That $\Delta\epsilon_n = \hat{\epsilon}_n - \epsilon_n$

$$
\begin{aligned}
P(\Delta\epsilon_n \leq -\tau) &= P(\frac{\Delta\epsilon_n - \mu}{\sigma} \leq \frac{-\tau - \mu}{\sigma}) && (5)\\
&= \Phi(\frac{-\tau - \mu}{\sigma}) && (6)\\
&= \Phi(\frac{-\tau + 2/n}{\sqrt{2}/n}) && (7)\\
&= \Phi(\frac{-n\tau + 2}{\sqrt{2}}) && (8)\\
& && (9)
\end{aligned}
$$

$$
\begin{aligned}
P(\Delta\epsilon_n \geq \tau) &= P(\frac{\Delta\epsilon_n - \mu}{\sigma} \geq \frac{\tau - \mu}{\sigma}) && (10)\\
&= 1 - P(\frac{\Delta\epsilon_n - \mu}{\sigma} < \frac{\tau - \mu}{\sigma}) && (11)\\
&= 1 - \Phi(\frac{\tau - \mu}{\sigma}) && (12)\\
&= 1 - \Phi(\frac{n\tau - 2}{\sqrt{2}}) && (13)
\end{aligned}
$$

Thus, when $n \to \infty$

$$
\begin{aligned}
\lim_{n\to\infty} P(\Delta\epsilon_n \leq -\tau) &= 0 && (14)\\
\lim_{n\to\infty} P(\Delta\epsilon_n \geq \tau) &= 0 && (15)
\end{aligned}
$$

This can be conluced to

$$\lim_{n\to\infty} P(|\hat{\epsilon}_n - \epsilon_n| \geq \tau) = 0$$

The estimator is *consistent*.

Problem 7.10

This problem illustrates the very poor (even paradoxical) performance of cross-validation with very small sample sizes. Consider the resubstitution and leave-one-out estimators $\hat{\epsilon}_n^r$ and $\hat{\epsilon}_n^l$ for the 3NN classification rule, with a sample of size $n = 4$ from a mixture of two equally-likely Gaussian populations $\Pi_0 \sim N_d(\mu_0, \Sigma)$

and $\Pi_1 \sim N_d(\mu_1, \Sigma)$. Assume that μ_0 and μ_1 are far enough apart to make $\delta = \sqrt{(\mu_1 - \mu_0)^T \Sigma^{-1} (\mu_1 = \mu_0)} \gg 0$ (in which case the Bayes error is $\epsilon_{\text{bay}} = \Phi(-\frac{\delta}{2}) \approx 0$).

(a)

For a sample S_n with $N_0 = N_1 = 2$, which occurs $P(N_0 = 2) = \binom{4}{2} 2^{-4} = 37.5\%$ of the time, show that $\epsilon_n \approx 0$ but $\hat{\epsilon}_n^l = 1$

If $N_0 = N_1 = 2$, the leave-one-out method removes one of the data point. The remaining points will have the majority label and have opposite label to the removed point (Figure 5). This flipping causes $\hat{\epsilon}^l = 1$.

Since two Gaussian population are far away from each other. The decidsion boundary is in the middle of two means, and there is little overlap between two distribution. Thus, when $\delta \gg 0$, $\epsilon_n \approx 0$.

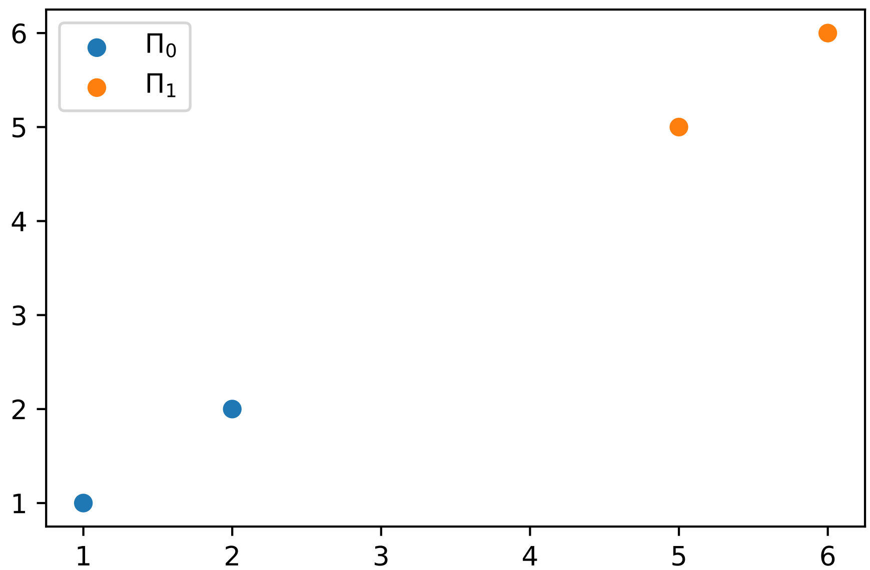


Figure 5: Two separated gaussian process in hyperplan with N0=N1=2

(b)

Show that $E[\epsilon_n] \approx \frac{5}{16} = 0.3125$, but $E[\hat{\epsilon}_n^l] = 0.5$, so that $\text{Bias}(\hat{\epsilon}_n^l) \approx \frac{3}{16} = 0.1875$, and the leave-one-out estimator is far from unbiased.

Given two label have equal occurrences,

- $P(N_0 = 0) = \binom{4}{0} 2^{-4} = 1 \cdot 2^{-4}$
  - $(N_0, N_1) = (0, 4)$
  - $\epsilon_n = \frac{1}{2}$ (always predicting N_1)
  - $\hat{\epsilon}_n^l = 0$
- $P(N_0 = 1) = \binom{4}{1} 2^{-4} = 4 \cdot 2^{-4}$
  - $(N_0, N_1) = (1, 3)$
  - $\epsilon_n = \frac{1}{2}$
  - $\hat{\epsilon}_n^l = \frac{1}{4}$
- $P(N_0 = 2) = \binom{4}{2} 2^{-4} = 6 \cdot 2^{-4}$
  - $(N_0, N_1) = (2, 2)$
  - $\epsilon_n = 0$
  - $\hat{\epsilon}_n^l = 1$ (flipped)
- $P(N_0 = 3) = \binom{4}{3} 2^{-4} = 4 \cdot 2^{-4}$
  - $(N_0, N_1) = (3, 1)$
  - $\epsilon_n = \frac{1}{2}$
  - $\hat{\epsilon}_n^l = \frac{1}{4}$
- $P(N_0 = 4) = \binom{4}{4} 2^{-4} = 1 \cdot 2^{-4}$
  - $(N_0, N_1) = (4, 0)$
  - $\epsilon_n = \frac{1}{2}$
  - $\hat{\epsilon}_n^l = 0$

$$E[\epsilon_n] = \frac{1}{2}\frac{1}{16} + \frac{1}{2}\frac{4}{16} + 0 + \frac{1}{2}\frac{4}{16} + \frac{1}{2}\frac{1}{16} = \frac{5}{16}$$

$$E[\hat{\epsilon}_n^l] = 0 + \frac{1}{4}\frac{4}{16} + 1\frac{6}{16} + \frac{1}{4}\frac{4}{16} + 0 = \frac{8}{16} = \frac{1}{2}$$

(c)

Show that $Var_d(\hat{\epsilon}_n^l) \approx \frac{103}{256} \approx 0.402$, which corresponds to a standard deviation of $\sqrt{0.402} = 0.634$. The leave-one-out estimator is therefore highly-biased and highly-variable in this case.

$$
\begin{aligned}
Var_d(\hat{\epsilon}_n^l) &= E[(\hat{\epsilon}_n^l - \epsilon_n)^2] - (E[\hat{\epsilon}_n^l - \epsilon_n])^2 && (16)\\
&= (0 - \frac{1}{2})^2 \frac{1}{16} + (\frac{1}{4} - \frac{1}{2})^2 \frac{4}{16} && (17)\\
&+ (1-0)^2 \frac{6}{16} + (\frac{1}{2} - \frac{1}{4})^2 \frac{4}{16} + (0 - \frac{1}{2})^2 \frac{1}{16} - (\frac{3}{16})^2 && (18)\\
&= 2(\frac{1}{2})^2 \frac{1}{16} + 2(\frac{1}{4})^2 \frac{4}{16} + \frac{6}{16} - (\frac{3}{16})^2 && (19)\\
&= \frac{14}{32} - (\frac{3}{16})^2 = \frac{103}{256} && (20)
\end{aligned}
$$

(d)

Consider the correlation coefficient of an error estimator $\hat{\epsilon}_n$ with the true error ϵ_n:

$$
\rho(\epsilon_n, \hat{\epsilon}_n) = \frac{Cov(\epsilon_n, \hat{\epsilon}_n)}{Std(\epsilon_n) Std(\hat{\epsilon}_n)}
$$

Show that $\rho(\epsilon_n, \hat{\epsilon}_n^l \approx 0.98)$, i.e., the leave-one-out estimator is almost perfectly negatively correlated with the true error.

$$
\begin{aligned}
Var(\hat{\epsilon}_n^l) &= E[\epsilon_n^2] - E[\epsilon_n]^2 && (21)\\
&= \frac{1}{16}\frac{4}{16} + \frac{6}{16} + \frac{1}{16}\frac{4}{16} = \frac{4+96+4}{256} - \frac{1}{4} = \frac{40}{256} = \frac{5}{32} && (22)
\end{aligned}
$$

$$
\begin{aligned}
Var(\epsilon_n) &= E[(\hat{\epsilon}_n^l)^2] - (E[\hat{\epsilon}_n^l])^2 && (23)\\
&= \frac{1}{4}\frac{1}{16} + \frac{1}{4}\frac{4}{16} && (24)\\
&+ \frac{1}{4}\frac{4}{16} + \frac{1}{4}\frac{1}{16} - (\frac{5}{16})^2 && (25)\\
&= \frac{10}{64} - \frac{25}{256} = \frac{15}{256} && (26)
\end{aligned}
$$

Use the previous results,

$$
\begin{aligned}
Cov(\epsilon_n, \hat{\epsilon}_n^l) &= E[\epsilon_n \hat{\epsilon}_n^l] - E[\epsilon_n]E[\hat{\epsilon}_n^l] && (27)\\
&= (0 + \frac{1}{2}\frac{1}{4}\frac{4}{16} + 0 + \frac{1}{2}\frac{1}{4}\frac{4}{16}) - \frac{5}{16}\frac{1}{2} && (28)\\
&= \frac{1}{16} - \frac{5}{32} = \frac{-3}{32} \approx -0.98 && (29)
\end{aligned}
$$

We can derive the correlation coefficient:

$$\rho(\epsilon_n, \hat{\epsilon}_n^l) = \frac{-3/32}{\sqrt{\frac{5}{32}}\sqrt{\frac{15}{256}}}$$

(e)

> For comparison, show that, although $E[\hat{\epsilon}_n^r] = \frac{1}{8} = 0.125$, so that $\text{Bias}(\hat{\epsilon}_n^r) \approx \frac{-3}{16} = -0.1875$, which is exactly the negative of the bias of leave-one-out, we have $Var_d(\hat{\epsilon}_n^r) \approx \frac{7}{256} \approx 0.027$, for a standard deviation of $\frac{\sqrt{7}}{16} \approx 0.165$, which is several times smaller than the leave-one-out variance, and $\rho(\epsilon_n, \hat{\epsilon}_n^r) \approx \sqrt{\frac{3}{5}} \approx 0.775$, showing that the resubstitution estimator is highly positively correlated with the true error.

The resubstitution error estimator uses 3 nearest neighbors, and no point is removed:

- $P(N_0 = 0) = \binom{4}{0}2^{-4} = 1 \cdot 2^{-4}$
  - $(N_0, N_1) = (0, 4)$
  - $\epsilon_n = \frac{1}{2}$
  - $\hat{\epsilon}_n^r = 0$
- $P(N_0 = 1) = \binom{4}{1}2^{-4} = 4 \cdot 2^{-4}$
  - $(N_0, N_1) = (1, 3)$
  - $\epsilon_n = \frac{1}{2}$
  - $\hat{\epsilon}_n^r = \frac{1}{4}$
- $P(N_0 = 2) = \binom{4}{2}2^{-4} = 6 \cdot 2^{-4}$
  - $(N_0, N_1) = (2, 2)$
  - $\epsilon_n = 0$
  - $\hat{\epsilon}_n^r = 0$
- $P(N_0 = 3) = \binom{4}{3}2^{-4} = 4 \cdot 2^{-4}$
  - $(N_0, N_1) = (3, 1)$
  - $\epsilon_n = \frac{1}{2}$
  - $\hat{\epsilon}_n^r = \frac{1}{4}$
- $P(N_0 = 4) = \binom{4}{4}2^{-4} = 1 \cdot 2^{-4}$
  - $(N_0, N_1) = (4, 0)$
  - $\epsilon_n = \frac{1}{2}$
  - $\hat{\epsilon}_n^r = 0$

The resubstitution estimator is positively correlated with the true error.

References

Braga-Neto, Ulisses. 2020. *Fundamentals of Pattern Recognition and Machine Learning*. Springer.

Problem 6.12

```python
import tensorflow as tf
import numpy as np
import PIL
import cv2
import os
import sklearn
import pandas as pd
import pickle
import platform
from tqdm.notebook import tqdm
from sklearn.multiclass import OneVsOneClassifier
from sklearn import preprocessing
from sklearn import svm
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
from scipy import stats as st
```

Computational Environment

```python
physical_devices = tf.config.list_physical_devices('GPU')
my_system = platform.uname()
print(physical_devices)
print(f"System: {my_system.system}")
print(f"Node Name: {my_system.node}")
print(f"Release: {my_system.release}")
print(f"Version: {my_system.version}")
print(f"Machine: {my_system.machine}")
print(f"Processor: {my_system.processor}")
```

```
[PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU')]
System: Darwin
Node Name: qiushaotings-MacBook-Pro-2.local
Release: 21.5.0
Version: Darwin Kernel Version 21.5.0: Tue Apr 26 21:08:29 PDT 2022; root:xnu-8020.121.3~4/R
Machine: arm64
Processor: i386
```

Helper function

```
def load_image(path, width=484, preprocess_input=tf.keras.applications.vgg16.preprocess_in
    """
    Load and Preprocessing image
    """
    img = tf.keras.utils.load_img(path)
    x = tf.keras.utils.img_to_array(img)
    x = x[0:width,:,:]
    x = np.expand_dims(x, axis=0)
    return tf.keras.applications.vgg16.preprocess_input(x)
```

Data inspection

```
dpath = os.path.join("data", "CMU-UHCS_Dataset")
pic_path = os.path.join(dpath, "images")
df_micro = pd.read_csv( os.path.join(dpath, "micrograph.csv"))
df_micro = df_micro[["path", "primary_microconstituent"]]

for i in range(0, len(df_micro)):
    img_ph = os.path.join(pic_path,df_micro.iloc[i][0])
    assert os.path.exists(img_ph)
    df_micro.iloc[i][0] = img_ph
df_micro2 = df_micro.copy()
CLS_rm = ["pearlite+widmanstatten", "martensite", "pearlite+spheroidite"] #(type, sample s
```

```
for c in CLS_rm:
    df_micro.drop(df_micro[df_micro["primary_microconstituent"] == c].index, inplace=True)
```

```
# labels
name_lbs = df_micro["primary_microconstituent"].unique()
le = preprocessing.LabelEncoder()
le.fit(name_lbs)
list(le.classes_)
```

```
['network', 'pearlite', 'spheroidite', 'spheroidite+widmanstatten']
```

```
dlabel = le.transform(df_micro["primary_microconstituent"])
df_micro.insert(2, "label", dlabel)
df_micro
```

	path	primary_microconstituent	label
0	data/CMU-UHCS_Dataset/images/micrograph1.tif	pearlite	1
1	data/CMU-UHCS_Dataset/images/micrograph2.tif	spheroidite	2
3	data/CMU-UHCS_Dataset/images/micrograph5.tif	pearlite	1
4	data/CMU-UHCS_Dataset/images/micrograph6.tif	spheroidite	2
5	data/CMU-UHCS_Dataset/images/micrograph7.tif	spheroidite+widmanstatten	3
...	...	...	...
955	data/CMU-UHCS_Dataset/images/micrograph1722.tif	spheroidite	2
957	data/CMU-UHCS_Dataset/images/micrograph1726.tif	spheroidite+widmanstatten	3
958	data/CMU-UHCS_Dataset/images/micrograph1730.png	spheroidite	2
959	data/CMU-UHCS_Dataset/images/micrograph1731.tif	pearlite	1
960	data/CMU-UHCS_Dataset/images/micrograph1732.tif	pearlite	1

Data Processing

```
# Train-test split
df_test = df_micro.copy()
df_train = pd.DataFrame(columns = df_micro.keys())

split_info = [("spheroidite", 100),\
              ("network", 100),\
              ("pearlite", 100),\
              ("spheroidite+widmanstatten", 60)] #(type, sample size)



for ln in split_info:
    label, n = ln
    id_train = df_micro[df_micro["primary_microconstituent"] == label][0:n].index
    df_test.drop(id_train, axis=0, inplace=True)
    df_train = pd.concat([df_train, df_micro.loc[id_train]])
```

```
df_train
```

	path	primary_microconstituent	label
1	data/CMU-UHCS_Dataset/images/micrograph2.tif	spheroidite	2
4	data/CMU-UHCS_Dataset/images/micrograph6.tif	spheroidite	2
8	data/CMU-UHCS_Dataset/images/micrograph10.png	spheroidite	2
9	data/CMU-UHCS_Dataset/images/micrograph11.tif	spheroidite	2
20	data/CMU-UHCS_Dataset/images/micrograph29.tif	spheroidite	2
...	...	...	...
596	data/CMU-UHCS_Dataset/images/micrograph1093.tif	spheroidite+widmanstatten	3
618	data/CMU-UHCS_Dataset/images/micrograph1129.tif	spheroidite+widmanstatten	3
631	data/CMU-UHCS_Dataset/images/micrograph1156.tif	spheroidite+widmanstatten	3
672	data/CMU-UHCS_Dataset/images/micrograph1218.tif	spheroidite+widmanstatten	3
673	data/CMU-UHCS_Dataset/images/micrograph1219.tif	spheroidite+widmanstatten	3

```
df_test
```

	path	primary_microconstituent	label
237	data/CMU-UHCS_Dataset/images/micrograph436.png	spheroidite	2
238	data/CMU-UHCS_Dataset/images/micrograph437.tif	spheroidite	2
239	data/CMU-UHCS_Dataset/images/micrograph440.png	spheroidite	2
241	data/CMU-UHCS_Dataset/images/micrograph442.tif	spheroidite	2
242	data/CMU-UHCS_Dataset/images/micrograph443.tif	spheroidite	2
...	...	...	...
955	data/CMU-UHCS_Dataset/images/micrograph1722.tif	spheroidite	2
957	data/CMU-UHCS_Dataset/images/micrograph1726.tif	spheroidite+widmanstatten	3
958	data/CMU-UHCS_Dataset/images/micrograph1730.png	spheroidite	2
959	data/CMU-UHCS_Dataset/images/micrograph1731.tif	pearlite	1
960	data/CMU-UHCS_Dataset/images/micrograph1732.tif	pearlite	1

Feature Extraction

```
# VGG16

base_model = tf.keras.applications.vgg16.VGG16(
    include_top=False,
    weights='imagenet',
    input_tensor=None,
    input_shape=None,
    pooling=None,
```

```python
    classes=1000,
    classifier_activation='softmax'
)

base_model.summary()
```

```
Model: "vgg16"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 input_1 (InputLayer)        [(None, None, None, 3)]   0

 block1_conv1 (Conv2D)       (None, None, None, 64)    1792

 block1_conv2 (Conv2D)       (None, None, None, 64)    36928

 block1_pool (MaxPooling2D)  (None, None, None, 64)    0

 block2_conv1 (Conv2D)       (None, None, None, 128)   73856

 block2_conv2 (Conv2D)       (None, None, None, 128)   147584

 block2_pool (MaxPooling2D)  (None, None, None, 128)   0

 block3_conv1 (Conv2D)       (None, None, None, 256)   295168

 block3_conv2 (Conv2D)       (None, None, None, 256)   590080

 block3_conv3 (Conv2D)       (None, None, None, 256)   590080

 block3_pool (MaxPooling2D)  (None, None, None, 256)   0

 block4_conv1 (Conv2D)       (None, None, None, 512)   1180160

 block4_conv2 (Conv2D)       (None, None, None, 512)   2359808

 block4_conv3 (Conv2D)       (None, None, None, 512)   2359808

 block4_pool (MaxPooling2D)  (None, None, None, 512)   0

 block5_conv1 (Conv2D)       (None, None, None, 512)   2359808
```

```
 block5_conv2 (Conv2D)       (None, None, None, 512)   2359808

 block5_conv3 (Conv2D)       (None, None, None, 512)   2359808

 block5_pool (MaxPooling2D)  (None, None, None, 512)   0

=================================================================
Total params: 14,714,688
Trainable params: 14,714,688
Non-trainable params: 0
_________________________________________________________________
```

Use five layers

```
out_layer_ns = ["block{}_pool".format(i) for i in range(1,6)]
out_layer_ns
```

```
['block1_pool', 'block2_pool', 'block3_pool', 'block4_pool', 'block5_pool']
```

```
# Construct 5 models for feature extraction
extmodel = dict(zip(out_layer_ns, [tf.keras.Model(
    inputs= base_model.input,
    outputs=base_model.get_layer(bk_name).output
) for bk_name in out_layer_ns]))

extmodel
```

```
{'block1_pool': <keras.engine.functional.Functional at 0x29f411e20>,
 'block2_pool': <keras.engine.functional.Functional at 0x2af72ecd0>,
 'block3_pool': <keras.engine.functional.Functional at 0x2b06b63d0>,
 'block4_pool': <keras.engine.functional.Functional at 0x2b06be5b0>,
 'block5_pool': <keras.engine.functional.Functional at 0x2b06bedf0>}
```

```
# Display output dimensions
out_shapes = [extmodel[m].output_shape[-1] for m in extmodel.keys()]
out_shapes
```

```
[64, 128, 256, 512, 512]
```

```python
# Initiate feature maps for testing and training
fs_train = [np.zeros((df_train.shape[0], n_f)) for n_f in out_shapes]
fs_test = [np.zeros((df_test.shape[0], n_f)) for n_f in out_shapes]

features_train = dict(zip(out_layer_ns, fs_train))
features_test = dict(zip(out_layer_ns, fs_test))

features_train
```

```
{'block1_pool': array([[0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        ...,
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.]]),
 'block2_pool': array([[0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        ...,
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.]]),
 'block3_pool': array([[0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        ...,
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.]]),
 'block4_pool': array([[0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        ...,
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.]]),
 'block5_pool': array([[0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        ...,
```

```
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.],
        [0., 0., 0., ..., 0., 0., 0.]])}
```

```
# Feature extraction with VGG16
if os.path.exists(os.path.join(dpath, "feature_train.pkl")) == False:
    for m in tqdm(extmodel.keys()):
        for i, df in enumerate([df_train, df_test]):
            for j, ph in tqdm(enumerate(df["path"])):
                x = load_image(ph)
                xb = extmodel[m].predict(x, verbose = 0) # silence output
                F = np.mean(xb,axis=(0,1,2))
                # Save features
                if i ==0:
                    features_train[m][j, :] = F
                else:
                    features_test[m][j, :] = F
    #save file
    paths =  dict(zip(["train", "test"],\
        [os.path.join(dpath, "feature_{}.pkl".format(n))\
         for n in ["train", "test"]]))
    ## Create new files
    f_train = open(paths["train"], "wb")
    f_test = open(paths["test"], "wb")
    ## Write
    pickle.dump(features_train, f_train)
    pickle.dump(features_test, f_test)
    ## Close files
    f_train.close()
    f_test.close()
```

SVM

```
# load data
ftn = open(paths["train"], "rb")
ftt = open(paths["test"], "rb")
featn = pickle.load(ftn) # train feature
featt = pickle.load(ftt) # test feature
ftn.close()
ftt.close()
```

```python
# label
ltrain = df_train[["primary_microconstituent", "label"]].reset_index()
ltest = df_test[["primary_microconstituent", "label"]].reset_index()
```

```python
ltrain
```

	index	primary_microconstituent	label
0	1	spheroidite	2
1	4	spheroidite	2
2	8	spheroidite	2
3	9	spheroidite	2
4	20	spheroidite	2
...	...	...	...
355	596	spheroidite+widmanstatten	3
356	618	spheroidite+widmanstatten	3
357	631	spheroidite+widmanstatten	3
358	672	spheroidite+widmanstatten	3
359	673	spheroidite+widmanstatten	3

```python
ltest["label"].to_numpy()
```

```
array([2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 2,
       0, 2, 2, 0, 2, 0, 2, 0, 2, 2, 2, 2, 2, 2, 0, 2, 2, 0, 2, 2, 2, 0,
       0, 0, 2, 2, 0, 2, 2, 0, 2, 0, 2, 2, 0, 0, 0, 0, 2, 0, 0, 2, 2, 2,
       2, 2, 0, 0, 2, 2, 0, 2, 2, 2, 2, 0, 2, 2, 0, 0, 2, 2, 2, 2, 0, 2,
       0, 2, 0, 2, 2, 2, 2, 2, 2, 0, 0, 0, 0, 0, 0, 2, 2, 2, 2, 2, 2, 0,
       0, 2, 2, 2, 2, 0, 0, 2, 2, 2, 2, 0, 2, 2, 2, 2, 2, 0, 2, 2, 2, 2,
       2, 2, 0, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 2, 2, 2, 2, 2, 2, 0, 0,
       2, 0, 2, 2, 0, 2, 0, 2, 2, 3, 0, 2, 2, 0, 3, 2, 2, 0, 0, 2, 0, 2,
       0, 2, 2, 2, 2, 0, 2, 3, 0, 2, 0, 2, 0, 3, 2, 0, 2, 0, 2, 2, 2, 3,
       2, 2, 0, 0, 2, 2, 0, 2, 2, 2, 3, 2, 0, 2, 0, 2, 2, 2, 2, 2, 2, 0,
       0, 2, 0, 2, 0, 0, 2, 0, 3, 0, 2, 2, 2, 2, 3, 3, 0, 2, 0, 0, 2, 0,
       0, 2, 2, 2, 0, 2, 1, 2, 0, 2, 2, 0, 0, 0, 3, 1, 3, 1, 0, 2, 2, 1,
       0, 2, 2, 2, 2, 0, 2, 2, 2, 2, 3, 2, 2, 0, 1, 1, 2, 1, 3, 3, 1, 2,
       2, 0, 3, 0, 2, 0, 2, 2, 2, 3, 0, 2, 2, 2, 0, 0, 3, 1, 1, 1, 0, 1,
```

```
       3, 0, 1, 2, 2, 3, 2, 2, 0, 2, 2, 0, 2, 0, 2, 2, 2, 1, 1, 2, 1, 2,
       2, 2, 1, 1, 0, 0, 2, 1, 2, 3, 2, 2, 2, 0, 2, 2, 2, 2, 1, 1, 0, 2,
       2, 0, 2, 2, 0, 0, 2, 1, 2, 3, 2, 1, 1])
```

```
clf.predict(featt["block1_pool"])
```

```
array([2, 3, 2, 1, 2, 1, 2, 3, 2, 2, 1, 2, 2, 2, 2, 2, 2, 1, 2, 2, 2, 2,
       2, 3, 0, 2, 2, 2, 2, 0, 2, 2, 2, 3, 2, 2, 1, 2, 1, 2, 3, 2, 3, 2,
       2, 2, 3, 2, 3, 2, 2, 3, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 3, 2, 2, 0,
       3, 2, 2, 0, 1, 1, 1, 2, 3, 2, 0, 0, 3, 0, 2, 2, 0, 0, 0, 0, 2, 2,
       3, 2, 1, 3, 2, 2, 0, 0, 2, 1, 2, 2, 2, 3, 0, 2, 2, 0, 3, 2, 2, 2,
       3, 3, 2, 2, 0, 2, 2, 3, 2, 2, 2, 2, 2, 0, 0, 3, 0, 3, 0, 2, 2, 0,
       2, 1, 2, 0, 2, 2, 3, 2, 1, 2, 2, 0, 2, 2, 0, 2, 2, 2, 2, 2, 2, 2,
       0, 2, 0, 0, 2, 2, 2, 2, 2, 0, 0, 0, 0, 0, 2, 0, 2, 1, 2, 2, 2, 2,
       0, 2, 2, 1, 2, 2, 0, 2, 2, 2, 0, 0, 3, 2, 2, 2, 2, 0, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 2, 2, 1, 3, 2, 2, 2, 2, 2, 1, 2, 0,
       2, 2, 3, 2, 0, 0, 2, 2, 2, 2, 0, 2, 2, 2, 2, 2, 2, 0, 2, 2, 0, 2,
       0, 0, 3, 2, 2, 0, 2, 3, 2, 2, 0, 2, 0, 3, 2, 2, 2, 2, 1, 3, 3, 0,
       1, 2, 2, 0, 0, 2, 0, 2, 3, 2, 2, 2, 0, 2, 0, 2, 2, 1, 2, 2, 2, 0,
       0, 2, 2, 2, 3, 2, 2, 0, 2, 0, 2, 2, 3, 0, 3, 1, 0, 2, 3, 2, 2, 2,
       2, 2, 3, 2, 0, 3, 2, 2, 0, 2, 2, 2, 2, 0, 3, 2, 1, 1, 3, 2, 2, 1,
       0, 1, 2, 2, 2, 0, 2, 2, 1, 0, 0, 1, 0, 0, 1, 1, 1, 0, 1, 3, 2, 2,
       2, 2, 1, 2, 2, 3, 2, 2, 2, 0, 2, 3, 0, 2, 0, 0, 3, 1, 1, 1, 0, 1,
       2, 2, 1, 0, 2, 2, 2, 0, 2, 2, 2, 2, 2, 0, 2, 2, 0, 1, 3, 2, 1, 2,
       2, 2, 2, 1, 2, 3, 2, 0, 2, 2, 2, 2, 0, 0, 1, 3, 0, 2, 1, 2, 3, 1,
       2, 2, 2, 2, 0, 0, 1, 1, 0, 3, 2, 1, 1])
```

One-to-One SVM

```
class One2OneSVM:
    def __init__(self, n_class=4):
        self.n_class = n_class
        self.clfs = [[svm.SVC(kernel="rbf", C=1., gamma="auto")\
                     for i in range(0,self.n_class)]\
                     for j in range(0,self.n_class)]
        self.cv = np.zeros((self.n_class,self.n_class))
    def train(self, ltrain, feature, fold=10):
        # traversal all features
        for i in range(0, self.n_class-1):
            lis = ltrain[ltrain["label"] == i].index.to_numpy()
```

```
            for j in range(i+1, self.n_class):
                ljs = ltrain[ltrain["label"] == j].index.to_numpy()
                # Data
                X = np.concatenate(\
                  (feature[lis,:],\
                   feature[ljs,:]), axis=0)
                Y = np.concatenate((np.ones(len(lis))*i,np.ones(len(ljs))*j))
                # Train SVM
                scores = sklearn.model_selection.cross_val_score(self.clfs[i][j], X, Y, cv
                self.clfs[i][j].fit(X,Y)
                self.cv[i][j] = np.max(scores)

    def test_1v1_error(self, ltest, feature):
        # traversal all features
        errM = np.zeros((self.n_class, self.n_class))
        for i in range(0, self.n_class-1):
            lis = ltest[ltest["label"] == i].index.to_numpy()
            for j in range(i+1, self.n_class):
                ljs = ltest[ltest["label"] == j].index.to_numpy()
                # Data
                X = np.concatenate(\
                  (feature[lis,:],\
                   feature[ljs,:]), axis=0)
                Y = np.concatenate((np.ones(len(lis))*i,np.ones(len(ljs))*j))
                # Train SVM
                y_pred = self.clfs[i][j].predict(X)
                errM[i,j] = error(Y, y_pred)
        return errM

    def predict(self, feature):
        predM = np.zeros(( int(self.n_class * (self.n_class -1)/2) , feature.shape[0]))
        c = 0
        for i in range(0, self.n_class-1):
            for j in range(i+1, self.n_class):
                predM[c,:] = self.clfs[i][j].predict(feature)
                c += 1
        return st.mode(predM, axis=0, keepdims=True).mode[0,:] #majority voting

def error(ans, pred):
    assert len(ans) == len(pred)
    return (ans != pred).sum()/float(ans.size)
```

(a)

The convolution layer used and the cross-validated error estimate for each of the six pairwise two-label classifiers

(b)

Separate test error rates on the unused micrographs of each of the four categories, for the pairwise two-label classifiers and the multilabel one-vs-one voting classifier described previously. For the pairwise classifiers use only the test micrographs with the two labels used to train the classifier. For the multilabel classifier, use the test micrographs with the corresponding four labels.

```
def df_cv(m, clf, info=""):
    var1 = []
    var2 = []
    cvs = []
    errs = []
    for i in range(0, m.shape[0]-1):
        for j in range(i+1, m.shape[0]):
            var1.append(i)
            var2.append(j)
            cvs.append(clf.cv[i,j])
            errs.append(m[i,j])
    infos = [info] * len(errs)
    return pd.DataFrame({"Info": infos, "Label 1": var1, "Label 2": var2, "Test error": er
```

Pair-wise classifier

```
df_errors = []
for b in out_layer_ns:
    clf1 = One2OneSVM()
    clf1.train(ltrain, features_train[b])
    errs = clf1.test_1v1_error(ltest, features_test[b])
    df_errors.append(df_cv(errs, clf1, b))

res_error = pd.concat(df_errors)
res_error
```

	Info	Label 1	Label 2	Test error	Cross Validation Score
0	block1_pool	0	1	0.823529	0.500
1	block1_pool	0	2	0.290155	0.550
2	block1_pool	0	3	0.157895	0.625
3	block1_pool	1	2	0.906040	0.500
4	block1_pool	1	3	0.466667	0.625
5	block1_pool	2	3	0.071186	0.625
0	block2_pool	0	1	0.823529	0.650
1	block2_pool	0	2	0.709845	0.650
2	block2_pool	0	3	0.157895	0.625
3	block2_pool	1	2	0.919463	0.500
4	block2_pool	1	3	0.466667	0.625
5	block2_pool	2	3	0.071186	0.625
0	block3_pool	0	1	0.823529	0.600
1	block3_pool	0	2	0.290155	0.600
2	block3_pool	0	3	0.157895	0.625
3	block3_pool	1	2	0.080537	0.550
4	block3_pool	1	3	0.466667	0.625
5	block3_pool	2	3	0.071186	0.625
0	block4_pool	0	1	0.823529	0.500
1	block4_pool	0	2	0.290155	0.550
2	block4_pool	0	3	0.157895	0.625
3	block4_pool	1	2	0.080537	0.500
4	block4_pool	1	3	0.466667	0.625
5	block4_pool	2	3	0.071186	0.625
0	block5_pool	0	1	0.073529	1.000
1	block5_pool	0	2	0.033679	1.000
2	block5_pool	0	3	0.060150	1.000
3	block5_pool	1	2	0.000000	1.000
4	block5_pool	1	3	0.088889	1.000
5	block5_pool	2	3	0.061017	0.875

Multiple one-vs-one classifier

```
# Multiclass one-vs-one
dfm_errors = []
for b in out_layer_ns:
    clf = OneVsOneClassifier(svm.SVC(kernel="rbf", C=1., gamma="auto").fit(features_train[
          ltrain["label"].to_numpy(int))
    clf.fit(features_train[b],\
```

```
            ltrain["label"].to_numpy(int))
    y_predm = clf.predict(features_test[b])
    dfm_errors.append(1 - error(y_predm, ltest["label"].to_numpy()))

# Display result
res_multi1v1 = pd.DataFrame({"Info": out_layer_ns, "Score": dfm_errors})
res_multi1v1
```

	Info	Score
0	block1_pool	0.064965
1	block2_pool	0.055684
2	block3_pool	0.635731
3	block4_pool	0.635731
4	block5_pool	0.928074

(c)

> For the mixed pearlite + spheroidite test micrographs, apply the trained pairwise classifier for pearlite vs. spheroidite and the multilabel voting classifier. Print the predicted labels by these two classifiers side by side (one row for each test micrograph). Comment your results

The pairwise SVM classifier performs better than Multiclass one-to-one classifier. Because the pairwise SVM is specialized for the binary problem and not be interfered with other classification setting.

```
ltestm = ltest[(ltest["primary_microconstituent"] == "pearlite") |\
      (ltest["primary_microconstituent"] == "spheroidite")]
feature_m = features_test["block5_pool"][ltestm.index.to_numpy(), :]
l = le.transform(["pearlite", "spheroidite"])

pred_pairs = clf1.clfs[l[0]][l[1]].predict(feature_m)
pred_multi = clf.predict(feature_m)

res_ps = pd.DataFrame({"Test Label": le.inverse_transform(ltestm["label"]),\
              "Pairwise (pearlite vs. spheroidite)": le.inverse_transform(pred_pairs.astyp
              "Multi-OnevsOne": le.inverse_transform(pred_multi)})

print(res_ps.to_string())
```

	Test Label	Pairwise (pearlite vs. spheroidite)	Multi-OnevsOne
0	spheroidite	spheroidite	spheroidite
1	spheroidite	spheroidite	spheroidite
2	spheroidite	spheroidite	spheroidite
3	spheroidite	spheroidite	spheroidite
4	spheroidite	spheroidite	spheroidite
5	spheroidite	spheroidite	spheroidite
6	spheroidite	spheroidite	spheroidite
7	spheroidite	spheroidite	spheroidite
8	spheroidite	spheroidite	spheroidite
9	spheroidite	spheroidite	spheroidite
10	spheroidite	spheroidite	spheroidite
11	spheroidite	spheroidite	spheroidite
12	spheroidite	spheroidite	spheroidite
13	spheroidite	spheroidite	spheroidite
14	spheroidite	spheroidite	spheroidite
15	spheroidite	spheroidite	spheroidite
16	spheroidite	spheroidite	spheroidite
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218	spheroidite	spheroidite	spheroidite+widmanstatten
219	pearlite	pearlite	pearlite
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233	spheroidite	spheroidite	network
234	spheroidite	spheroidite	spheroidite
235	spheroidite	spheroidite	spheroidite+widmanstatten
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253	pearlite	pearlite	pearlite
254	pearlite	pearlite	pearlite
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256	pearlite	pearlite	pearlite

257	spheroidite	spheroidite	spheroidite
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267	pearlite	pearlite	pearlite
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287	pearlite	pearlite	pearlite
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292	spheroidite	spheroidite	spheroidite
293	pearlite	pearlite	pearlite
294	spheroidite	spheroidite	spheroidite
295	spheroidite	spheroidite	spheroidite
296	pearlite	pearlite	pearlite
297	pearlite	pearlite	pearlite

(d)

> Now apply the multilabel classifier on the pearlite + Widmanst¨atten and martensite micrographs and print the predicted labels. Compare to the results in part (c)

There is no specific relation for these unseen datasets. The prediction can not extrapolate, and (c) has preferred prediction accuracy and consistency.

```
df_micro2 = df_micro2[(df_micro2["primary_microconstituent"] == "pearlite+widmanstatten")
(df_micro2["primary_microconstituent"] == "martensite")]

# Encode labels
le2 = preprocessing.LabelEncoder()
le2.fit(df_micro2["primary_microconstituent"].unique())
list(le2.classes_)
```

```
['martensite', 'pearlite+widmanstatten']
```

```
dlabel2 = le2.transform(df_micro2["primary_microconstituent"])
df_micro2.insert(2, "label", dlabel2)
```

```
df_micro2
```

	path	primary_microconstituent	label
15	data/CMU-UHCS_Dataset/images/micrograph20.tif	martensite	0
29	data/CMU-UHCS_Dataset/images/micrograph41.tif	martensite	0
31	data/CMU-UHCS_Dataset/images/micrograph44.tif	martensite	0
63	data/CMU-UHCS_Dataset/images/micrograph99.tif	martensite	0
71	data/CMU-UHCS_Dataset/images/micrograph114.tif	martensite	0
...	...	...	...
892	data/CMU-UHCS_Dataset/images/micrograph1599.tif	martensite	0
936	data/CMU-UHCS_Dataset/images/micrograph1684.tif	pearlite+widmanstatten	1
942	data/CMU-UHCS_Dataset/images/micrograph1697.tif	martensite	0
944	data/CMU-UHCS_Dataset/images/micrograph1700.tif	martensite	0
956	data/CMU-UHCS_Dataset/images/micrograph1723.tif	martensite	0

```
# Feature extraction with VGG16
if os.path.exists(os.path.join(dpath, "feature_test2.pkl")) == False:
    fs_test2 = np.zeros((df_micro2.shape[0], out_shapes[-1]))
    m = "block5_pool"
    for j, ph in tqdm(enumerate(df_micro2["path"])):
        x = load_image(ph)
        xb = extmodel[m].predict(x, verbose = 0) # silence output
        F = np.mean(xb,axis=(0,1,2))
        # Save features
        fs_test2[j, :] = F

    # Save data
    ## Create new files
    fs_test2_p = open(os.path.join(dpath, "feature_test2.pkl"), "wb")
    ## Write
    pickle.dump(fs_test2, fs_test2_p)
    ## Close files
    fs_test2_p.close()
```

```
#load data
fs_test2_p  = open(os.path.join(dpath, "feature_test2.pkl"), "rb")
fs_test2 = pickle.load(fs_test2_p) # train feature
fs_test2_p .close()
```

```
pred_multi2 = clf.predict(fs_test2)

res_ps2 = pd.DataFrame({"Test Label": le2.inverse_transform(df_micro2["label"]),\
              "Multi-OnevsOne": le.inverse_transform(pred_multi2)})

print(res_ps2.to_string())
```

```
                Test Label           Multi-OnevsOne
0               martensite              spheroidite
1               martensite                  network
2               martensite                 pearlite
3               martensite              spheroidite
4               martensite              spheroidite
5               martensite                  network
6               martensite              spheroidite
7   pearlite+widmanstatten                 pearlite
```

8	martensite	pearlite
9	martensite	spheroidite
10	martensite	spheroidite
11	pearlite+widmanstatten	pearlite
12	martensite	pearlite
13	pearlite+widmanstatten	pearlite
14	martensite	pearlite
15	pearlite+widmanstatten	spheroidite
16	pearlite+widmanstatten	spheroidite+widmanstatten
17	pearlite+widmanstatten	pearlite
18	martensite	pearlite
19	pearlite+widmanstatten	spheroidite
20	pearlite+widmanstatten	pearlite
21	pearlite+widmanstatten	spheroidite
22	pearlite+widmanstatten	spheroidite
23	pearlite+widmanstatten	pearlite
24	pearlite+widmanstatten	pearlite
25	martensite	pearlite
26	martensite	spheroidite
27	martensite	pearlite
28	martensite	spheroidite
29	martensite	pearlite
30	martensite	spheroidite
31	martensite	pearlite
32	pearlite+widmanstatten	pearlite
33	martensite	pearlite
34	martensite	spheroidite
35	pearlite+widmanstatten	spheroidite
36	martensite	spheroidite
37	pearlite+widmanstatten	spheroidite
38	pearlite+widmanstatten	pearlite
39	pearlite+widmanstatten	pearlite
40	martensite	pearlite
41	martensite	spheroidite
42	pearlite+widmanstatten	pearlite
43	pearlite+widmanstatten	spheroidite
44	pearlite+widmanstatten	spheroidite+widmanstatten
45	pearlite+widmanstatten	pearlite
46	pearlite+widmanstatten	pearlite
47	martensite	pearlite
48	pearlite+widmanstatten	pearlite
49	martensite	pearlite
50	pearlite+widmanstatten	spheroidite+widmanstatten

51	pearlite+widmanstatten	pearlite
52	martensite	pearlite
53	pearlite+widmanstatten	spheroidite
54	martensite	spheroidite
55	martensite	spheroidite
56	martensite	pearlite
57	martensite	network
58	martensite	spheroidite
59	pearlite+widmanstatten	pearlite
60	martensite	spheroidite
61	martensite	pearlite
62	martensite	spheroidite