

# exercise\_sheet\_9

June 21, 2022

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12.5/25 points

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## 0.1 Exercise sheet 9

### 0.1.1 Exercise 1 - Ensemble Learning (8 points) 4/8

```
[1]: import pandas as pd
import numpy as np

from sklearn.datasets import make_classification
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold
from sklearn.model_selection import GridSearchCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.linear_model import Lasso
```

1. Using the `titanic_survival_dataset.csv`, train the following (scikit-learn) models using nested cross validation while optimizing a selected number of hyperparameters in the inner loop using grid search, then compute the probabilities of the outcomes:

```
[2]: dataset = pd.read_csv('titanic_survival_data.csv')
dataset
```

```
[2]:
```

	PassengerId	Pclass	Sex	Age	SibSp	Parch	Fare	Embarked	\
0	1	3	0	22.0	1	0	7.2500	0	
1	2	1	1	38.0	1	0	71.2833	1	
2	3	3	1	26.0	0	0	7.9250	0	
3	4	1	1	35.0	1	0	53.1000	0	
4	5	3	0	35.0	0	0	8.0500	0	
..	...	...	...	...	...	...	...		
886	887	2	0	27.0	0	0	13.0000	0	
887	888	1	1	19.0	0	0	30.0000	0	
888	889	3	1	24.0	1	2	23.4500	0	
889	890	1	0	26.0	0	0	30.0000	1	
890	891	3	0	32.0	0	0	7.7500	2	

	no_cabin	Label
0	2	0
1	1	1
2	2	1
3	1	1
4	2	0
..	...	...
886	2	0
887	1	1
888	2	0
889	1	1
890	2	0

[891 rows x 10 columns]

a. Random forest, optimizing the number of estimators (1 point)

```
[3]: # Divide the dataframe into target and rest
X = dataset.drop(['Label'], axis=1)
y = dataset['Label']

# We configure the nested cross-validation procedure: we are going to have a
↳ outer loop and a inner loop
# Outer loop: helps us asses the quality of the model
cv_outer = KFold(n_splits=5, shuffle=True, random_state=1)

# Inner loop: for model/parameter selection
cv_inner = KFold(n_splits=4, shuffle=True, random_state=1)

# We define the model
model = RandomForestClassifier(random_state=1)

# We define search space: we want to optimize the number of estimators
↳ (parameter grid)
space = dict()
space['n_estimators'] = [10, 100, 250, 500]

# Define search
search = GridSearchCV(model, space, scoring='accuracy', n_jobs=1, cv=cv_inner,
↳ refit=True)

# We fit the search to be able to find best hyperparameters
result = search.fit(X, y)

# Execute the nested cross-validation
```

```

scores = cross_val_score(search, X, y, scoring='accuracy', cv=cv_outer,
    ↪n_jobs=-1)

# Report performance
print('Accuracy: %.3f (%.3f)' % (np.mean(scores), np.std(scores)))
print(f'The best option is using {result.best_params_} with a {result.
    ↪best_score_} accuracy')

```

Accuracy: 0.814 (0.031)

The best option is using {'n\_estimators': 250} with a 0.8159718013978103 accuracy

```

[4]: # Divide the dataset into 80% training and 20% test
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20,
    ↪random_state=1)

# Compute the probability of the outcomes
prob1 = result.predict_proba(X_test)
print(prob1[:10])

```

0.5/1

The gridsearch() already splits the data with cv.  
Why split it again?

```

[[0.028 0.972]
 [0.964 0.036]
 [0.048 0.952]
 [0.692 0.308]
 [0.008 0.992]
 [0.98 0.02 ]
 [0.796 0.204]
 [0.016 0.984]
 [0.916 0.084]
 [0.064 0.936]]

```

b. Gradient boosting, optimizing boosting steps (2 point)

```

[5]: # Divide the dataframe into target and rest
X = dataset.drop(['Label'], axis=1)
y = dataset['Label']

# We configure the nested cross-validation procedure: we are going to have a
    ↪outer loop and a inner loop
# Outer loop: helps us asses the quality of the model
cv_outer = KFold(n_splits=5, shuffle=True, random_state=1)

# Inner loop: for model/parameter selection
cv_inner = KFold(n_splits=4, shuffle=True, random_state=1)

# We define the model

```

```

model = GradientBoostingClassifier(random_state=1)

# We define search space: we want to optimize the number of estimators
↳ (parameter grid)
# N_estimators = the number of boosting stages to perform
space = dict()
space['n_estimators'] = [50, 100, 250, 500]

# Define search
search = GridSearchCV(model, space, scoring='accuracy', cv=cv_inner, refit=True)

# We fit the search to be able to find best hyperparameters
result = search.fit(X, y)

# Execute the nested cross-validation
scores = cross_val_score(result, X, y, cv=cv_outer, scoring='accuracy')

# Report performance
print('Accuracy: %.3f (%.3f)' % (np.mean(scores), np.std(scores)))
print(f'The best option is using {result.best_params_} with a {result.
↳ best_score_} accuracy')

```

Accuracy: 0.827 (0.033)

The best option is using {'n\_estimators': 50} with a 0.8148759746293379 accuracy

```

[6]: X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20,
↳ random_state=1)

# Compute the probability of the outcomes
prob2 = result.predict_proba(X_test)
print(prob2[:10])

```

Same as above  
1/2

```

[[0.09832013 0.90167987]
 [0.89106083 0.10893917]
 [0.14291704 0.85708296]
 [0.47774111 0.52225889]
 [0.06326413 0.93673587]
 [0.89173272 0.10826728]
 [0.83131371 0.16868629]
 [0.03892631 0.96107369]
 [0.72615598 0.27384402]
 [0.32831925 0.67168075]]

```

c. Lasso penalized logistic regression, optimizing L1 regularization strength (1 point)

```

[7]: # Divide the dataframe into target and rest
X = dataset.drop(['Label'], axis=1)
y = dataset['Label']

```

```

# We configure the nested cross-validation procedure: we are going to have a
↳ outer loop and a inner loop
# Outer loop: helps us asses the quality of the model
cv_outer = KFold(n_splits=5, shuffle=True, random_state=1)

# Inner loop: for model/parameter selection
cv_inner = KFold(n_splits=4, shuffle=True, random_state=1)

# We define the model
model = Lasso(random_state=1)
# Lasso is a linear model. We asked for logistic regression with lasso penalization

# We define search space: we want to optimize the L1 regularization strength,
↳ which is alpha
space = dict()
space['alpha'] = [1, 5, 10, 15]
# Define search
search = GridSearchCV(model, space, cv=cv_inner, refit=True)

# We fit the search to be able to find best hyperparameters
result = search.fit(X, y)

# Execute the nested cross-validation
scores = cross_val_score(result, X, y, cv=cv_outer)

# Report performance
print(f'The best option is using {result.best_params_}')

```

The best option is using {'alpha': 1}

I know we can't use the predict\_proba method, instead we should use the CalibratedClassifierCV but I'm not able to implement it.

## 2. Inform yourself about calibration curves (reliability diagrams).

1/1

d. Describe how calibration curves can explain your model's performance. (1 point)

Calibration curves or reliability diagrams compare the calibration of classifier's probabilities.

We usually used accuracy to measure a model's performance, however a model should also be well-calibrated.

This calibration plot is going to show the relation between the true class of the samples and the predicted probabilities. Therefore, this will give us a measure of how realistic a model prediction is.

e. Use the predicted probabilities of each model from question 1 to plot a calibration curve, then explain your results. (3 points)

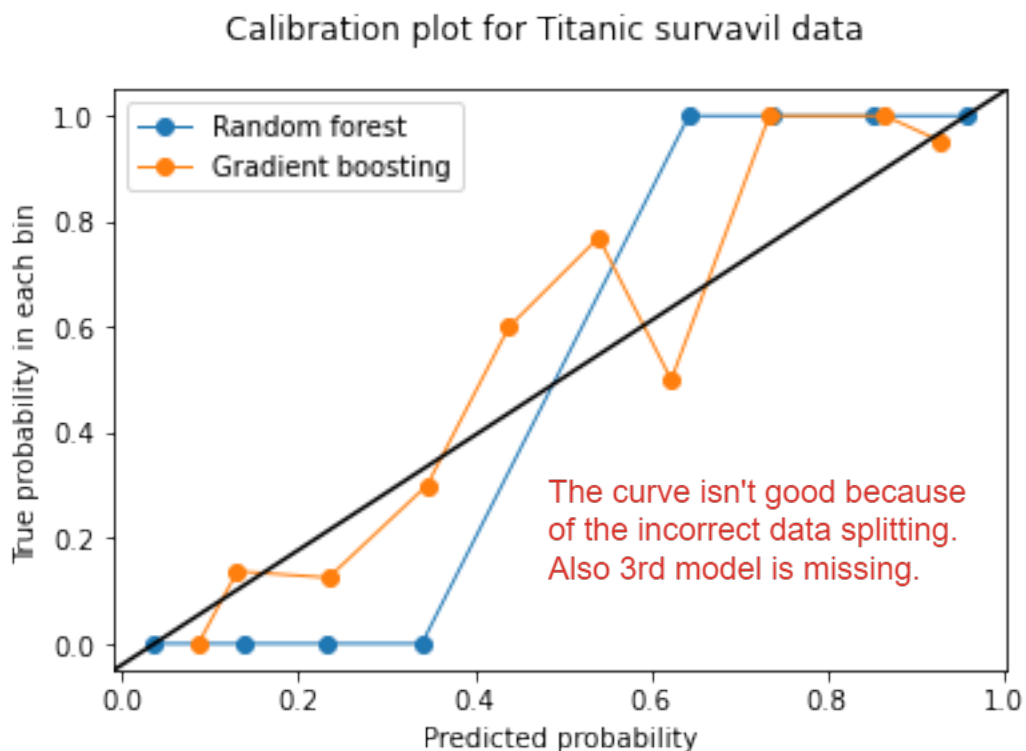
```
[8]: import matplotlib.pyplot as plt
from sklearn.calibration import calibration_curve

rf_y, rf_x = calibration_curve(y_test, prob1[:,1], n_bins=10)
gb_y, gb_x = calibration_curve(y_test, prob2[:,1], n_bins=10)
```

```
[9]: import matplotlib.pyplot as plt
import matplotlib.lines as mlines
import matplotlib.transforms as mtransforms

fig, ax = plt.subplots()
# only these two lines are calibration curves
plt.plot(rf_x, rf_y, marker='o', linewidth=1, label='Random forest')
plt.plot(gb_x, gb_y, marker='o', linewidth=1, label='Gradient boosting')

# reference line, legends, and axis labels
line = mlines.Line2D([0, 1], [0, 1], color='black')
transform = ax.transAxes
line.set_transform(transform)
ax.add_line(line)
fig.suptitle('Calibration plot for Titanic survavil data')
ax.set_xlabel('Predicted probability')
ax.set_ylabel('True probability in each bin')
plt.legend()
plt.show()
```



1.5/3

We could say the model trained with Gradient Boosting is performing best than Random Forest. Nevertheless, it is not a great performance either.

---

exercise2)

8.5/10

1. Suppose there is a Multi-Layer Perceptron (MLP) composed of one input layer with 8 neurons, followed by one hidden layer with 30 artificial neurons, and one output layer with 3 artificial neurons. All artificial neurons use the ReLU activation function.
  - a. Deduce the shape of input matrix X, hidden layer's weight vector Wh, bias vector bh and the shape of the network's output matrix Y. (2 points)

shape of input matrix X = number of neurones \* batch size  
X = 8 \* batch size

Hidden layer's weight vector Wh = 240

1.5/2

Hidden layer's bias vector bh = 30

shape of the network's output matrix Y = batch size \* number of neurones in output layer

- b. Write the equation that computes the network's output matrix Y as a function of X, Wh, bh, Wo and bo. (2 points)

$Y = (bo + Wo) * (bh + whX)$

2/2

$Y = 93(30 + 1920 \text{ batch size})$

2. What are the principal and unavoidable limitations of the backpropagation (BP)? (1 point)

-It relies on input to perform on a specific problem

-It is sensitive to complex/ noisy data

-It needs the derivatives of activation functions for the network design time.

0.5/1

principle?  
The limitation is also incomplete.

---

3-4) Compute h1, h2, o1, and total error using ReLU units. (2 points)

```
[10]: from sklearn.metrics import mean_squared_error

def relu(x):
    return max(0.0, x)

i1, i2 = 0.9, 0.3
w1, w2, w3, w4, w5, w6 = -0.2, 0.35, 0.12, 0.8, 0.45, 0.5
b1, b2, b3 = 0.15, -0.2, 0.5

h1_prev = w1*i1 + w2*i2 + b1
h2_prev = w3*i1 + w4*i2 + b2
```

```

h1_net = relu(h1_prev)
h2_net = relu(h2_prev)
o1 = w5*h1_net + w6*h2_net + b3
total_error = mean_squared_error([1], [o1])

print("h1: ", h1_net)
print("h2: ", h2_net)
print("o1: ", o1)
print("total_error: ", total_error)

```

2/2

```

h1: 0.07499999999999997
h2: 0.14799999999999996
o1: 0.60775
total_error: 0.15386006249999998

```

- 5) Calculate the updates of the network weights  $w_1, \dots, w_6$  and bias terms  $b_1, b_2, b_3$  using backpropagation. Assume a learning rate of 1 for the sake of simplicity. (3 points).

derivative of relu is defined as;

Don't forget that,

2.5/3

$f(x) = 1$  if  $x > 0$   $f(x) = 0$  if  $x \leq 0$

$$\frac{\partial L}{\partial o} = -2 * (1 - o1)$$

New value = old value - step size

```

[11]: par_L_over_w6 = -2*(1 - o1)*1*h2_prev
      par_L_over_w6

```

```
[11]: -0.11610599999999997
```

$$\frac{\partial L}{\partial w6} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial w6} = -2 * (1 - o1) * \text{relu}'(h1) * h2 = -0.1161$$

```

[12]: par_L_over_w5 = -2*(1 - o1)*1*h1_prev
      par_L_over_w5

```

```
[12]: -0.05883749999999997
```

$$\frac{\partial L}{\partial w5} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial w5} = -2 * (1 - o1) * \text{relu}'(h1) * h1 = -0.0588$$

```

[13]: par_L_over_b3 = -2*(1 - o1)*1
      par_L_over_b3

```

```
[13]: -0.7845
```

$$\frac{\partial L}{\partial b3} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial b3} = -2 * (1 - o1) * b3 = -0.7845$$

```

[14]: par_L_over_w1 = -2*(1 - o1)*1*w5*i1
      par_L_over_w1

```

```
[14]: -0.31772249999999996
```



$$\frac{\partial L}{\partial w1} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial h1} * \frac{\partial h1}{\partial w1} = -2 * (1 - o1) * w5 * \text{relu}'(h1) * i1 = -0.3177$$

```
[15]: par_L_over_w2 = -2*(1 - o1)*1*w5*i2
      par_L_over_w2
```

[15]: -0.10590749999999999

$$\frac{\partial L}{\partial w2} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial h1} * \frac{\partial h1}{\partial w2} = -2 * (1 - o1) * w5 * \text{relu}'(h1) * i2 = -0.1059$$

```
[16]: par_L_over_w3 = -2*(1 - o1)*1*w6*i1
      par_L_over_w3
```

[16]: -0.353025

$$\frac{\partial L}{\partial w3} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial h1} * \frac{\partial h1}{\partial w3} = -2 * (1 - o1) * w6 * \text{relu}'(h1) * i1 = -0.3530$$

```
[17]: par_L_over_w4 = -2*(1 - o1)*1*w6*i2
      par_L_over_w4
```

[17]: -0.11767499999999999

$$\frac{\partial L}{\partial w4} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial h1} * \frac{\partial h1}{\partial w4} = -2 * (1 - o1) * w6 * \text{relu}'(h1) * i2 = -0.1176$$

```
[18]: par_L_over_b2 = -2*(1 - o1)*1*w6
      par_L_over_b2
```

[18]: -0.39225

$$\frac{\partial L}{\partial b2} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial b2} = -2 * (1 - o1) * w6 * \text{relu}'(h1) = -0.3922$$

```
[19]: par_L_over_b1 = -2*(1 - o1)*1*w5
      par_L_over_b1
```

[19]: -0.353025

$$\frac{\partial L}{\partial b1} = \frac{\partial L}{\partial o1} * \frac{\partial o1}{\partial b1} = -2 * (1 - o1) * w5 * \text{relu}'(h1) = -0.3530$$


---