In [1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline

from sklearn.neural_network import MLPClassifier
from sklearn.metrics import mean_squared_error, classification_report, confusion_matrix, f1_score, precision_score, rec
from sklearn.model_selection import train_test_split

from collections import Counter
```

Data

This data is actually related to the elastic strain engineering task: given the (modified) deformation tensor, predict, whether the tiny diamond crystal under this deformation is a direct-bandgap semiconductor, or not.

I will save you some time and process the data for you.

In [2]:
```
df = pd.read_csv('c_gw_direct.csv')
```

In [3]:
```
df.shape
```

Out[3]:
```
(9766, 7)
```

In [4]:
```
df
```

Out[4]:

	exx	exy	exz	eyz	eyy	ezz	is_direct
0	-0.049931	0.019480	-0.012549	0.071484	0.000141	0.036242	False
1	0.057604	0.070671	-0.010140	-0.063918	0.032494	-0.078462	False
2	-0.020174	-0.059848	0.017878	0.077713	-0.087613	-0.079651	False
3	-0.023523	-0.026120	0.045459	-0.035286	-0.000705	0.038353	False
4	-0.050925	-0.006037	-0.042681	-0.016254	-0.019372	-0.037559	False
...	...	...	...	...	...	...	...
9761	-0.096821	0.049679	-0.065829	0.060488	0.008918	0.006889	False
9762	-0.074071	0.027148	-0.056629	-0.068732	0.070384	-0.008722	False
9763	-0.061505	0.015496	0.077352	-0.037589	-0.047513	-0.045182	False
9764	-0.037760	0.037480	0.002881	-0.059958	-0.047096	0.060803	False
9765	0.017428	0.008733	0.099832	0.028535	-0.054355	-0.006599	False

9766 rows × 7 columns

In [5]:
```
df.is_direct.sum()
```

Out[5]:
```
1376
```

In [6]:
```
# Getting arrays from table
X = df[['exx', 'exy', 'exz', 'eyz', 'eyy', 'ezz']].values
y = df['is_direct'].ravel()
```

In [7]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.2,
                                                    random_state=124)

Counter(y_train)
```

Out[7]:
```
Counter({False: 6723, True: 1089})
```

(3 pts) Train and evaluate a simple neural network classifier

- Train a model
- Calculate its precision, recall, f1-score
- Take a look at the confusion matrix

Train a model

In [47]:
```
model = MLPClassifier(max_iter=10000)
model.fit(X_train, y_train)
```

Out[47]:
```
MLPClassifier(max_iter=10000)
```

Look at the metrics

In [48]:
```
predictions = model.predict(X_test)

precision = precision_score(y_test, predictions)
print(f'Precision: {precision}')

recall = recall_score(y_test, predictions)
print(f'Recall: {recall}')

f1 = f1_score(y_test, predictions)
print(f'f1-score: {f1}')
```

```
Precision: 0.7883817427385892
Recall: 0.662020905923345
f1-score: 0.7196969696969697
```

Print the confusion matrix

In [10]:
```
confusion_matrix(y_test, predictions)
```

Out[10]:
```
array([[1623,   44],
       [ 137,  150]])
```

Итоги

- Recall 0.66 показывает, что модель в среднем обнаруживает класс в 66% случаев. Это лишь немного лучше, чем 50% угадывание.
- f1-score будем использовать как некую метрику, характеризующую баланс между precision и recall. Здесь за счет неплохой точности (precision) предсказания в целом f1-score повышается.
- Нужно искать метод для повышения precision и recall.

(3 pts) Use an undersampling technique to balance classes

- Balance training sample
- Train new model with the same hyperparameters as before
- Evaluate its metrics. Is is better than the original model?

In [49]:
```
idx_for_larger_class = np.nonzero(y_train == False)[0]
idx_for_smaller_class = np.nonzero(y_train == True)[0]

less_idx_for_larger_class = np.random.choice(idx_for_larger_class,
                                             len(idx_for_smaller_class),
                                             replace=False)

new_idx = list(less_idx_for_larger_class) + list(idx_for_smaller_class)

X_train_new = X_train[new_idx, :]
y_train_new = y_train[new_idx]

model_balanced = MLPClassifier(max_iter=10000)
model_balanced.fit(X_train_new, y_train_new)
```

Out[49]:
```
MLPClassifier(max_iter=10000)
```

In [50]:
```
predictions_balanced = model_balanced.predict(X_test)

precision = precision_score(y_test, predictions_balanced)
print(f'Precision: {precision}')

recall = recall_score(y_test, predictions_balanced)
print(f'Recall: {recall}')

f1 = f1_score(y_test, predictions_balanced)
print(f'f1-score: {f1}')
```

```
Precision: 0.5155642023346303
Recall: 0.9233449477351916
f1-score: 0.66167290886392
```

In [51]:
```
confusion_matrix(y_test, predictions_balanced)
```

Out[51]:
```
array([[1418,  249],
       [  22,  265]])
```

Итоги

- За счет большей сбалансированности данных модель стала лучше отличать один класс от другого. Об этом свидетельствует увеличение значения recall.
- Точность предсказания при этом уменьшилась. Это можно связать с уменьшением выборки, что в целом негативно влияет на обобщаемость модели.
- f1-score уменьшился на 0.05, поэтому вердикт следующий: случайная балансировка на данной выборке показывает плохие результаты.

(3 pts) Try the imblearn package and its undersampling methods

https://imbalanced-learn.org/stable/under_sampling.html

- Try NearMiss, NeighbourhoodCleaningRule, and EditedNearestNeighbours methods
- Do they perform better than the random undersampling?

You may need to reinstall sklearn if it is old

In [52]:
```
# !pip uninstall -v scikit-learn -y
```

In [53]:
```
# !pip install -v scikit-learn
```

In [54]:
```
# !pip install imblearn
```

In [55]:
```
from imblearn.under_sampling import NearMiss, EditedNearestNeighbours, NeighbourhoodCleaningRule
```

Balancing with NearMiss

In [56]:
```
nm1 = NearMiss(version=1)
X_resampled_nm1, y_resampled_nm1 = nm1.fit_resample(X_train, y_train)
```

In [57]:
```
model_balanced_nearmiss = MLPClassifier(max_iter=10000)
model_balanced_nearmiss.fit(X_resampled_nm1, y_resampled_nm1)
```

Out[57]:
```
MLPClassifier(max_iter=10000)
```

In [58]:
```
predictions_balanced_nearmiss = model_balanced_nearmiss.predict(X_test)

precision = precision_score(y_test, predictions_balanced_nearmiss)
print(f'Precision: {precision}')

recall = recall_score(y_test, predictions_balanced_nearmiss)
print(f'Recall: {recall}')

f1 = f1_score(y_test, predictions_balanced_nearmiss)
print(f'f1-score: {f1}')
```

```
Precision: 0.534521158129176
Recall: 0.8362369337979094
f1-score: 0.6521739130434783
```

Balancing with NeighbourhoodCleaningRule

In [59]:
```
ncr = NeighbourhoodCleaningRule()
X_resampled_ncr, y_resampled_ncr = ncr.fit_resample(X_train, y_train)
```

In [60]:
```
model_balanced_ncr = MLPClassifier(max_iter=10000)
model_balanced_ncr.fit(X_resampled_ncr, y_resampled_ncr)
```

Out[60]:
```
MLPClassifier(max_iter=10000)
```

In [61]:
```
predictions_balanced_ncr = model_balanced_ncr.predict(X_test)

precision = precision_score(y_test, predictions_balanced_ncr)
print(f'Precision: {precision}')

recall = recall_score(y_test, predictions_balanced_ncr)
print(f'Recall: {recall}')

f1 = f1_score(y_test, predictions_balanced_ncr)
print(f'f1-score: {f1}')
```

```
Precision: 0.6755852842809364
Recall: 0.7038327526132404
f1-score: 0.6894197952218429
```

Balancing with EditedNearestNeighbours

In [62]:
```
enn = EditedNearestNeighbours()
X_resampled_enn, y_resampled_enn = enn.fit_resample(X_train, y_train)
```

In [63]:
```
model_balanced_enn = MLPClassifier(max_iter=10000)
model_balanced_enn.fit(X_resampled_enn, y_resampled_enn)
```

Out[63]:
```
MLPClassifier(max_iter=10000)
```

In [64]:
```
predictions_balanced_enn = model_balanced_enn.predict(X_test)

precision = precision_score(y_test, predictions_balanced_enn)
print(f'Precision: {precision}')

recall = recall_score(y_test, predictions_balanced_enn)
print(f'Recall: {recall}')

f1 = f1_score(y_test, predictions_balanced_enn)
print(f'f1-score: {f1}')
```

```
Precision: 0.25
Recall: 0.010452961672473868
f1-score: 0.020066889632107024
```

Итоги

- NearMiss и NeighbourhoodCleaningRule дают результат хуже, чем без балансировки. Применение этих методов дает свои результаты, но в итоге f1-score не увеличивается, поэтому их использование здесь не оправданно.
- EdintedNearestNeighbours показывает колоссально негативный результат, метрики говорят сами за себя. Не рекомендую здесь.

(3 pts) Perform hyperparameter tuning

- Run a cycle through some hyperparater settings in order to find the best ones
- E.g. hidden layer sizes, alpha regularization ...
- You need to be able to outperform your initial model
- I do not care whether you use balanced or imbalanced training set

In [65]:
```
hidden_layer_sizes_list = [
    (200, ),
    (100, ),
    (100, 100, ),
    (50, 50, ),
    (50, 50, 50, ),
    (50, 50, 50, 50),
]

alpha_list = [
    0.000001, 0.00001, 0.0001, 0.001, 0.01,
]
```

In [66]:
```
metrics_grid = {
    'hidden_layer_sizes': [],
    'alpha': [],
    'precision': [],
    'recall': [],
    'f1': [],
}

for hidden_layer_sizes_ in hidden_layer_sizes_list:
    for alpha_ in alpha_list:
        model = MLPClassifier(hidden_layer_sizes=hidden_layer_sizes_, alpha=alpha_, max_iter=10000)
        model.fit(X_train, y_train)
        predictions = model.predict(X_test)

        precision = precision_score(y_test, predictions)
        recall = recall_score(y_test, predictions)
        f1 = f1_score(y_test, predictions)

        metrics_grid['hidden_layer_sizes'].append(hidden_layer_sizes_)
        metrics_grid['alpha'].append(alpha_)
        metrics_grid['precision'].append(precision)
        metrics_grid['recall'].append(recall)
        metrics_grid['f1'].append(f1)
```

```
/home/ilyavoronov/miniconda3/envs/plasma_env/lib/python3.9/site-packages/sklearn/metrics/_classification.py:1318: Undefi
nedMetricWarning: Precision is ill-defined and being set to 0.0 due to no predicted samples. Use `zero_division` paramet
er to control this behavior.
  _warn_prf(average, modifier, msg_start, len(result))
/home/ilyavoronov/miniconda3/envs/plasma_env/lib/python3.9/site-packages/sklearn/metrics/_classification.py:1318: Undefi
nedMetricWarning: Precision is ill-defined and being set to 0.0 due to no predicted samples. Use `zero_division` paramet
```

```
er to control this behavior.
  _warn_prf(average, modifier, msg_start, len(result))
/home/ilyavoronov/miniconda3/envs/plasma_env/lib/python3.9/site-packages/sklearn/metrics/_classification.py:1318: UndefinedMetricWarning: Precision is ill-defined and being set to 0.0 due to no predicted samples. Use `zero_division` parameter to control this behavior.
  _warn_prf(average, modifier, msg_start, len(result))
```

In [70]:

```python
metrics_grid_df = pd.DataFrame.from_dict(metrics_grid)
metrics_grid_df
```

Out[70]:

	hidden_layer_sizes	alpha	precision	recall	f1
0	(200,)	0.000001	0.851301	0.797909	0.823741
1	(200,)	0.000010	0.806897	0.815331	0.811092
2	(200,)	0.000100	0.890688	0.766551	0.823970
3	(200,)	0.001000	0.862745	0.766551	0.811808
4	(200,)	0.010000	0.714286	0.261324	0.382653
5	(100,)	0.000001	0.832579	0.641115	0.724409
6	(100,)	0.000010	0.741784	0.550523	0.632000
7	(100,)	0.000100	0.757991	0.578397	0.656126
8	(100,)	0.001000	0.816832	0.574913	0.674847
9	(100,)	0.010000	0.000000	0.000000	0.000000
10	(100, 100)	0.000001	0.832776	0.867596	0.849829
11	(100, 100)	0.000010	0.862676	0.853659	0.858144
12	(100, 100)	0.000100	0.880000	0.843206	0.861210
13	(100, 100)	0.001000	0.893939	0.822300	0.856624
14	(100, 100)	0.010000	0.837545	0.808362	0.822695
15	(50, 50)	0.000001	0.888462	0.804878	0.844607
16	(50, 50)	0.000010	0.871698	0.804878	0.836957
17	(50, 50)	0.000100	0.796552	0.804878	0.800693
18	(50, 50)	0.001000	0.886364	0.815331	0.849365
19	(50, 50)	0.010000	0.000000	0.000000	0.000000
20	(50, 50, 50)	0.000001	0.876812	0.843206	0.859680
21	(50, 50, 50)	0.000010	0.857664	0.818815	0.837790
22	(50, 50, 50)	0.000100	0.956938	0.696864	0.806452
23	(50, 50, 50)	0.001000	0.897233	0.790941	0.840741
24	(50, 50, 50)	0.010000	0.908333	0.759582	0.827324
25	(50, 50, 50, 50)	0.000001	0.887597	0.797909	0.840367
26	(50, 50, 50, 50)	0.000010	0.882353	0.783972	0.830258
27	(50, 50, 50, 50)	0.000100	0.596603	0.979094	0.741425
28	(50, 50, 50, 50)	0.001000	0.000000	0.000000	0.000000
29	(50, 50, 50, 50)	0.010000	0.972477	0.738676	0.839604

In [68]:

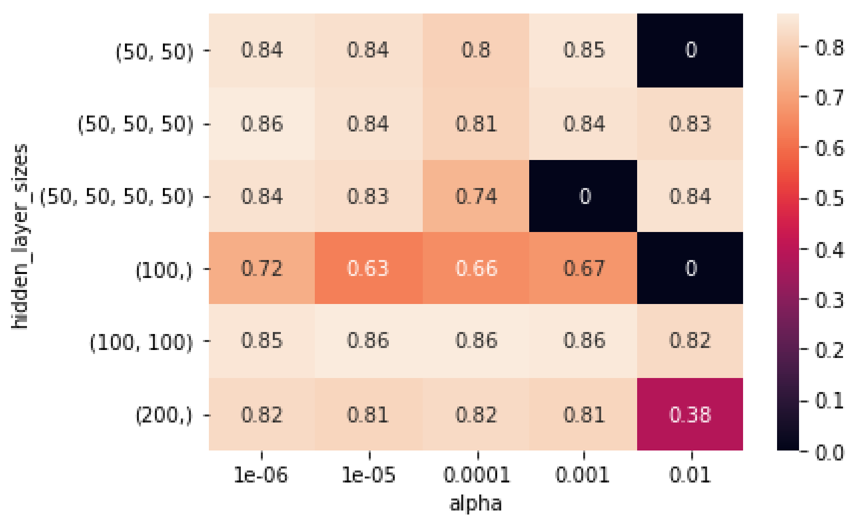
```python
pivot = metrics_grid_df.pivot_table(
    index=['hidden_layer_sizes'],
    columns=['alpha'],
    values='f1')
```

In [69]:

```python
sns.heatmap(pivot, annot=True)
```

Out[69]:

```
<AxesSubplot:xlabel='alpha', ylabel='hidden_layer_sizes'>
```



Итоги

- По сводной таблице видно, что с уменьшением alpha и увеличением числа слоев растет f1-score. Далее уже при повышении числа нейронов в слое тоже идет повышение. Но в то же время это ведет к увеличению расчетного времени.
- Лучше всего показали себя модели с размером (50, 50, 50) и (100, 100). Но последней для достижения этого уровня потребовался меньший параметр регуляризации.
- Оптимальной предлагается считать модель со слеудющими гипер-параметрами:

In [72]:

```
metrics_grid_df.loc[12]
```

Out[72]:

```
hidden_layer_sizes    (100, 100)
alpha                     0.0001
precision                   0.88
recall                  0.843206
f1                       0.86121
Name: 12, dtype: object
```

My final mark is $\min(mark, 10)$

In [ ]: