Chapter 3 - Fine-Tuning Your Model

Classification metrics

Accuracy: fraction of correctly classified samples

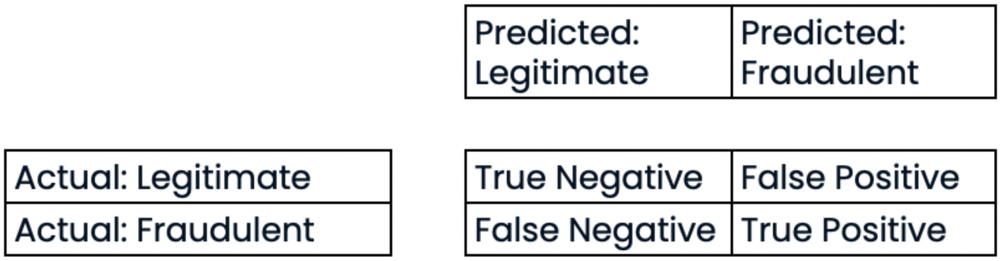
But not good for imbalanced classes (could just always predict majority class and couldn't identify e.g. fraudulent transactions)

Need to use confusion matrix (TN, FP, FN, TP)

In [2]:

```python
from IPython.display import Image
Image(filename='images/cf.png', width=500)
```

Out[2]:



	Predicted: Legitimate	Predicted: Fraudulent
Actual: Legitimate	True Negative	False Positive
Actual: Fraudulent	False Negative	True Positive

Accuracy = $\frac{tp+tn}{tp+tn+fp+fn}$

Precision ('positive predictive value') = $\frac{tp}{tp+fp}$

- High precision = lower false positive rate (e.g. not many legitimate transactions are predicted to be fraudulent)
- Concerns all predicted fraudulent +ve class (e.g. all predicted to be fraudulent)
- Right column of confusion matrix

Recall ('sensitivity') = $\frac{tp}{tp+fn}$

- High recall = lower false negative rate (e.g. predicted most fraudulent transactions correctly)
- Concerns all actual +ve class (e.g. all actual fraudulent)

F1 score = $2 * \frac{precision*recall}{precision+recall}$

- Harmonic mean of precision and recall
- Gives equal weights to precision and recall
- Favours models with similar precision and recall

In [1]:

```python
from sklearn.metrics import classification_report, confusion_matrix
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import train_test_split
import pandas as pd
```

In [2]:

```python
diabetes_df = pd.read_csv('./datasets/diabetes_clean.csv')
```

In [3]:

```python
diabetes_df_sub = diabetes_df[['bmi', 'age', 'diabetes']]
```

In [4]:
```
X_train, X_test, y_train, y_test = train_test_split(
    diabetes_df_sub.drop("diabetes", axis=1).values,
    diabetes_df_sub["diabetes"].values,
    test_size=0.3,
    random_state=42
)
```

In [5]:
```
knn = KNeighborsClassifier(n_neighbors=6)
knn.fit(X_train, y_train)
```

Out[5]:
```
▾           KNeighborsClassifier
KNeighborsClassifier(n_neighbors=6)
```

In [6]:
```
y_pred = knn.predict(X_test)
```

In [7]:
```
# Generate confusion matrix and classification report
print(confusion_matrix(y_test, y_pred)) # can add labels=[1,0] - careful of ordering!
print(classification_report(y_test, y_pred))
```

```
[[117  34]
 [ 47  33]]
              precision    recall  f1-score   support

           0       0.71      0.77      0.74       151
           1       0.49      0.41      0.45        80

    accuracy                           0.65       231
   macro avg       0.60      0.59      0.60       231
weighted avg       0.64      0.65      0.64       231
```

We see 117 TN, 34 FP, 47 FN and 33 TP. We see a better F1-score for the zero class (i.e. people without diabetes).

Precision (1): TP/(TP+FP) = 33/(33+34) = 0.49

Precision (0): TN/(TN+FN) = 117/(117+47) = 0.71

Recall (1): TP/(TP+FN) = 33/(33+47) = 0.41

Recall (0): TN/(TN+FP) = 117/(117+34) = 0.77

F1 (1): (2*(pr+re))/(pre+rec) = 0.45

F1 (0): (2*(pr+re))/(pre+rec) = 0.74

Accuracy: (TP+TN)/(TP+TN+FP+FN) = (33+117)/(33+117+34+47) = 0.65

Logistic regression and the ROC curve

Logistic regression:

- Used for classification problems
- Outputs probabilities:
    - If $p > 0.5$: data labeled 1

  - If $p < 0.5$: data labeled 0
- Produces a linear decision boundary

In [8]:

```
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import roc_curve
from sklearn.metrics import roc_auc_score
import matplotlib.pyplot as plt
```

In [9]:

```
X = diabetes_df.drop('diabetes', axis=1).values
y = diabetes_df['diabetes'].values
```

In [10]:

```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.3, random_state=42)
```

In [11]:

```
logreg = LogisticRegression()
logreg.fit(X_train, y_train)
```

```
/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/python3.
9/site-packages/sklearn/linear_model/_logistic.py:444: ConvergenceWarning: lbfgs failed
to converge (status=1):
STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

Increase the number of iterations (max_iter) or scale the data as shown in:
    https://scikit-learn.org/stable/modules/preprocessing.html
Please also refer to the documentation for alternative solver options:
    https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression
  n_iter_i = _check_optimize_result(
```

Out[11]:

```
▾ LogisticRegression

LogisticRegression()
```

In [12]:

```
y_pred_probs = logreg.predict_proba(X_test)[:, 1]
y_pred_probs[:10]
```

Out[12]:

```
array([0.26551021, 0.18336638, 0.1211966 , 0.15613521, 0.4961118 ,
       0.4458219 , 0.01359249, 0.61646093, 0.55640529, 0.79311776])
```

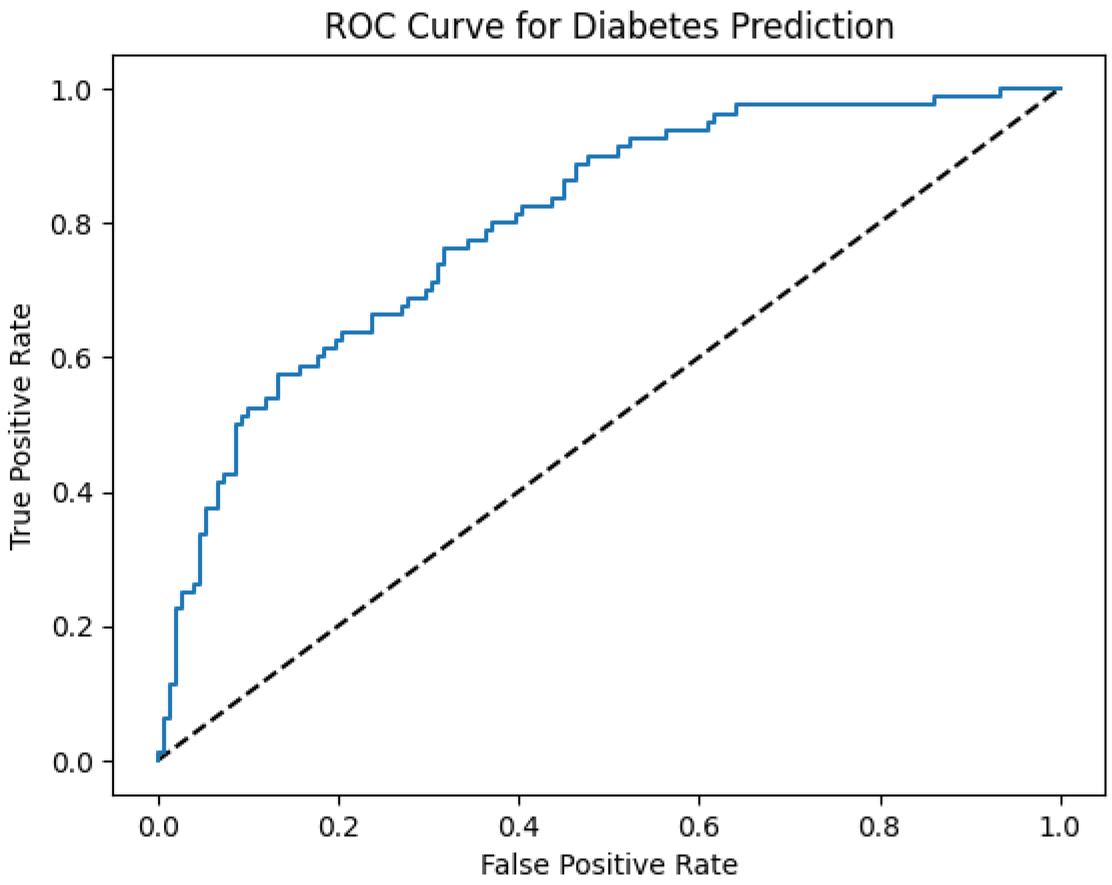
Probability of a diabetes diagnosis for the first 10 individuals ranges from 0.01 to 0.79.

In [13]:

```
# Generate ROC curve values: fpr, tpr, thresholds
fpr, tpr, thresholds = roc_curve(y_test, y_pred_probs)
```

In [14]:

```
plt.plot([0, 1], [0, 1], 'k--')
plt.plot(fpr, tpr)
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curve for Diabetes Prediction')
plt.show()
```



The model is much better than randomly guessing the class of each observation (ROC curve is above the dotted line, where the dotted line is a chance model - randomly guesses labels).

By default, logistic regression has a 0.5 threshold (can vary the threshold).

TPR = Recall = Sensitivity

FPR = 1 - Specificity = $1 - \frac{FP}{FP+TN}$

- If threshold=0: model predicts 1 for all observations, so predicts all +ve values correctly, and incorrectly predicts all -ve values (top right of ROC curve)
- If threshold=1: model predicts 0 for all data, so TPR and FPR = 0 (bottom left of ROC curve)
- If threshold=0.5: model above chance model line

Line is smoothed over different thresholds, which give different TPR and FPR values

ROC AUC: area under the curve (from 0-1, where 1 is ideal)

Perfect model: TPR=1, FPR=0

In [15]:
```
print(roc_auc_score(y_test, y_pred_probs))
print(confusion_matrix(y_test, y_pred))
print(classification_report(y_test, y_pred))
```

```
0.8002483443708608
[[117  34]
 [ 47  33]]
              precision    recall  f1-score   support

           0       0.71      0.77      0.74       151
           1       0.49      0.41      0.45        80

    accuracy                           0.65       231
   macro avg       0.60      0.59      0.60       231
weighted avg       0.64      0.65      0.64       231
```

ROC AUC score of 0.8002 means this model is 0.8002/0.5=60% better than a chance model at correctly predicting labels.

Hyperparameter tuning

Hyperparameters: parameters we specify before fitting the model (e.g. alpha and n_neighbors)

We try different hyperparameter values, fit all of them separately, see how well they perform, and choose the best performing values.

It's essential to use cross-validation to avoid overfitting to the test set (here we split the data and perform CV on the training set, and leave the test set for final evaluation).

In [16]:

```python
from sklearn.model_selection import GridSearchCV, RandomizedSearchCV
from sklearn.linear_model import Lasso
from sklearn.model_selection import KFold
import numpy as np
```

In [17]:

```python
param_grid = {"alpha": np.linspace(0.00001, 1, 20)}
```

In [18]:

```python
lasso = Lasso()
```

In [19]:

```python
kf = KFold()
```

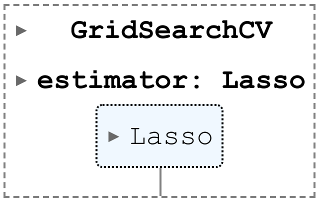
In [20]:

```python
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42)
```

In [21]:

```python
lasso_cv = GridSearchCV(lasso, param_grid, cv=kf)
lasso_cv.fit(X_train, y_train)
```

Out[21]:



In [22]:

```python
print("Tuned lasso paramaters: {}".format(lasso_cv.best_params_))
print("Tuned lasso score: {}".format(lasso_cv.best_score_))
```

```
Tuned lasso paramaters: {'alpha': 1e-05}
Tuned lasso score: 0.27122338337314245
```

We see the best model only has an R-squared score of 0.27 (using the optimal hyperparameters does not guarantee a high performing model).

Limitations of grid search: 10-fold CV, 3 hyperparameters, 30 total values = 900 fits! (can be computationally expensive)

In [23]:

```
params = {"penalty": ['l1', "l2"],
         "tol": np.linspace(0.0001, 1.0, 50),
         "C": np.linspace(0.1, 1.0, 50),
         "class_weight": ["balanced", {0: 0.8, 1: 0.2}]}
```

In [24]:

```
logreg = LogisticRegression()
```

In [25]:

```
logreg_cv = RandomizedSearchCV(logreg, params, cv=kf)
logreg_cv.fit(X_train, y_train)
```

```
/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/python3.
9/site-packages/sklearn/linear_model/_logistic.py:444: ConvergenceWarning: lbfgs failed
to converge (status=1):
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Increase the number of iterations (max_iter) or scale the data as shown in:
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/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/python3.
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```

```
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/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/python3.
9/site-packages/sklearn/linear_model/_logistic.py:444: ConvergenceWarning: lbfgs failed
to converge (status=1):
```

```
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    https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression
  n_iter_i = _check_optimize_result(
/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/python3.
9/site-packages/sklearn/model_selection/_validation.py:378: FitFailedWarning:
35 fits failed out of a total of 50.
The score on these train-test partitions for these parameters will be set to nan.
If these failures are not expected, you can try to debug them by setting error_score='ra
ise'.

Below are more details about the failures:
--------------------------------------------------------------------------------
35 fits failed with the following error:
Traceback (most recent call last):
  File "/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/
python3.9/site-packages/sklearn/model_selection/_validation.py", line 686, in _fit_and_s
core
    estimator.fit(X_train, y_train, **fit_params)
  File "/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/
python3.9/site-packages/sklearn/linear_model/_logistic.py", line 1091, in fit
    solver = _check_solver(self.solver, self.penalty, self.dual)
  File "/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/
python3.9/site-packages/sklearn/linear_model/_logistic.py", line 61, in _check_solver
    raise ValueError(
ValueError: Solver lbfgs supports only 'l2' or 'none' penalties, got l1 penalty.

  warnings.warn(some_fits_failed_message, FitFailedWarning)
/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/python3.
9/site-packages/sklearn/model_selection/_search.py:953: UserWarning: One or more of the
test scores are non-finite: [       nan        nan        nan        nan        nan 0.75
077969
        nan 0.70522458        nan 0.75243236]
  warnings.warn(
/Users/harrybaines/Documents/Coding/DataCamp-ML-Scientist-Track/datacampenv/lib/python3.
9/site-packages/sklearn/linear_model/_logistic.py:444: ConvergenceWarning: lbfgs failed
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Please also refer to the documentation for alternative solver options:
    https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression
  n_iter_i = _check_optimize_result(
```

Out[25]:

```
▸ RandomizedSearchCV
▸ estimator: LogisticRegression
    ▸ LogisticRegression
```

In [26]:

```
print("Tuned Logistic Regression Parameters: {}".format(logreg_cv.best_params_))
print("Tuned Logistic Regression Best Accuracy Score: {}".format(logreg_cv.best_score_))
```

```
Tuned Logistic Regression Parameters: {'tol': 0.9387816326530612, 'penalty': 'l2', 'clas
s_weight': 'balanced', 'C': 0.9081632653061225}
Tuned Logistic Regression Best Accuracy Score: 0.7524323603891777
```

In [27]:

```
test_score = logreg_cv.score(X_test, y_test)
test_score
```

Out[27]:

```
0.6948051948051948
```

After trying a few hyperparameters, we get a model with 70% accuracy!

In [ ]:

```
```