How good is your model?

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Classification metrics

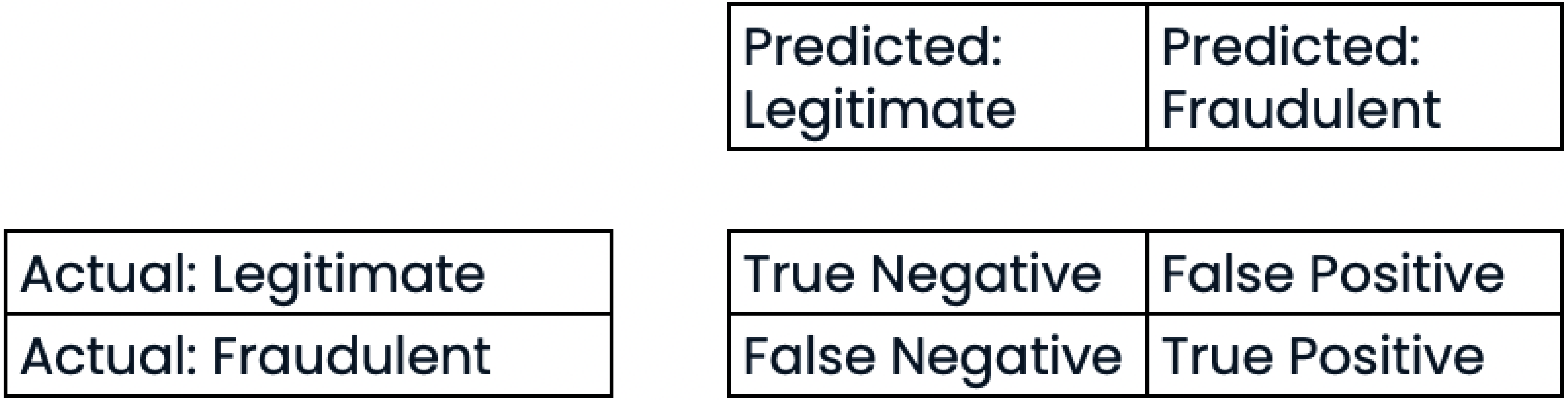
- Measuring model performance with accuracy:
  - Fraction of correctly classified samples
  - Not always a useful metric

Class imbalance

- Classification for predicting fraudulent bank transactions
  - 99% of transactions are legitimate; 1% are fraudulent
- Could build a classifier that predicts NONE of the transactions are fraudulent
  - 99% accurate!
  - But terrible at actually predicting fraudulent transactions
  - Fails at its original purpose
- Class imbalance: Uneven frequency of classes
- Need a different way to assess performance

Confusion matrix for assessing classification performance

- Confusion matrix



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

Assessing classification performance

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

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Assessing classification performance

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

- Accuracy:

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

Precision

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

- Precision

$$\frac{true\ positives}{true\ positives + false\ positives}$$

- High precision = lower false positive rate
- High precision: Not many legitimate transactions are predicted to be fraudulent

Recall

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

- Recall

$$\frac{true\ positives}{true\ positives + false\ negatives}$$

- High recall = lower false negative rate
- High recall: Predicted most fraudulent transactions correctly

F1 score

- F1 Score: $2 * \frac{precision * recall}{precision + recall}$

Confusion matrix in scikit-learn

```
from sklearn.metrics import classification_report, confusion_matrix
knn = KNeighborsClassifier(n_neighbors=7)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.4,
                                                    random_state=42)
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
```

Confusion matrix in scikit-learn

```
print(confusion_matrix(y_test, y_pred))
```

```
[[1106   11]
 [ 183   34]]
```

Classification report in scikit-learn

```python
print(classification_report(y_test, y_pred))
```

```
              precision    recall  f1-score   support

           0       0.86      0.99      0.92      1117
           1       0.76      0.16      0.26       217

    accuracy                           0.85      1334
   macro avg       0.81      0.57      0.59      1334
weighted avg       0.84      0.85      0.81      1334
```

Logistic regression and the ROC curve

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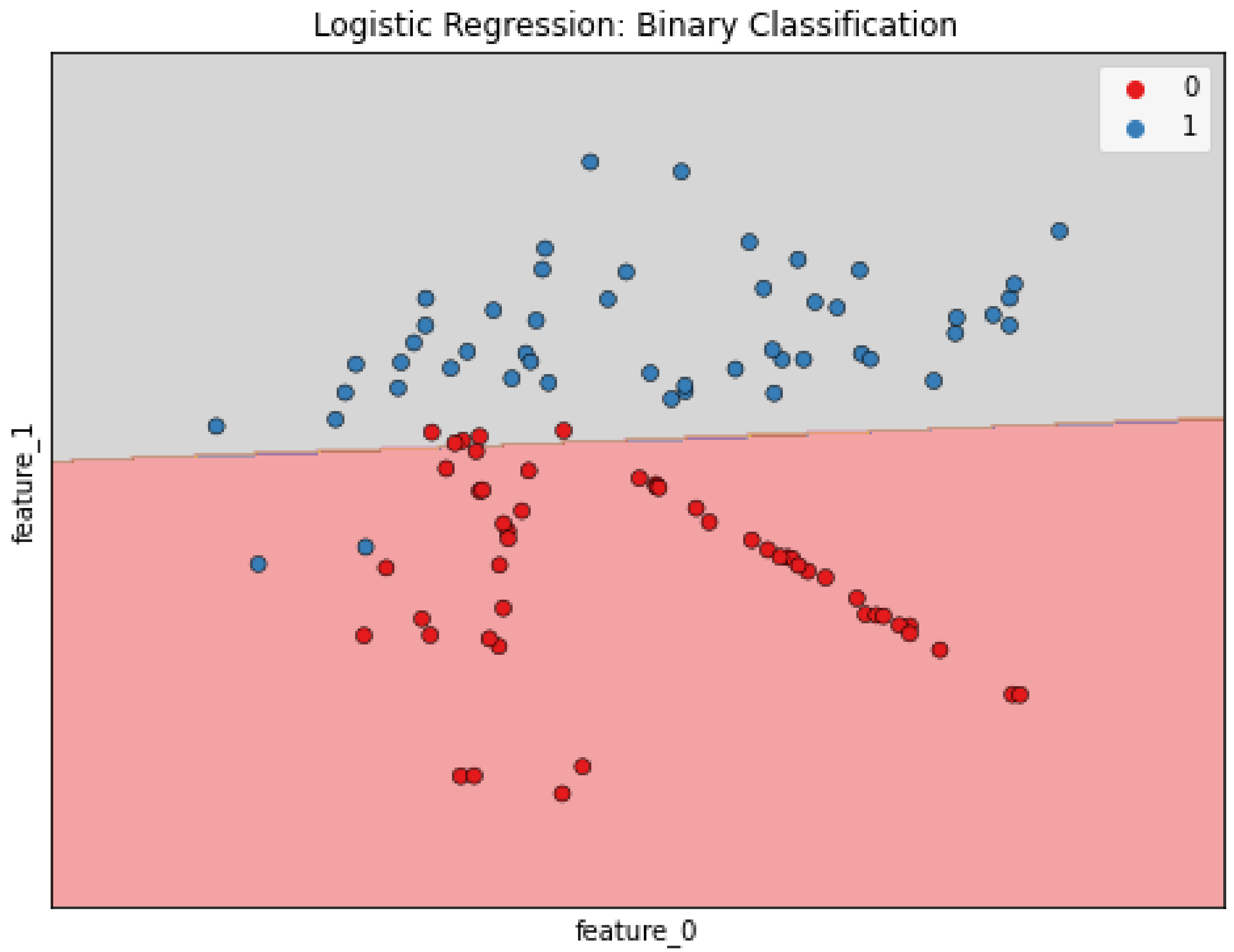
Logistic regression for binary classification

- Logistic regression is used for classification problems
- Logistic regression outputs probabilities
- If the probability, $p > 0.5$:
  - The data is labeled `1`
- If the probability, $p < 0.5$:
  - The data is labeled `0`

Linear decision boundary



Logistic regression in scikit-learn

```python
from sklearn.linear_model import LogisticRegression
logreg = LogisticRegression()
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
                                                    random_state=42)
logreg.fit(X_train, y_train)
y_pred = logreg.predict(X_test)
```

Predicting probabilities

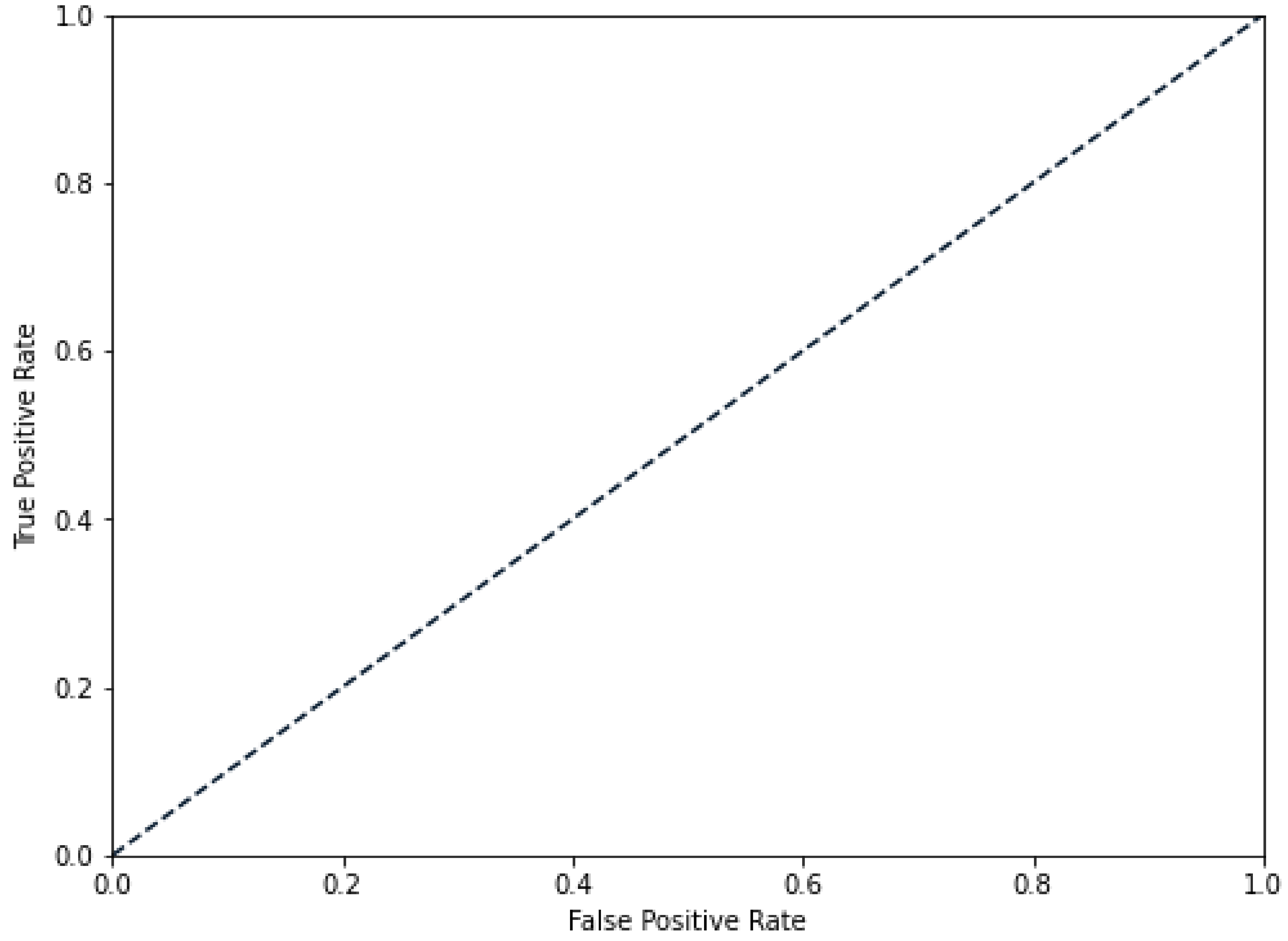
```
y_pred_probs = logreg.predict_proba(X_test)[:, 1]
print(y_pred_probs[0])
```

```
[0.08961376]
```

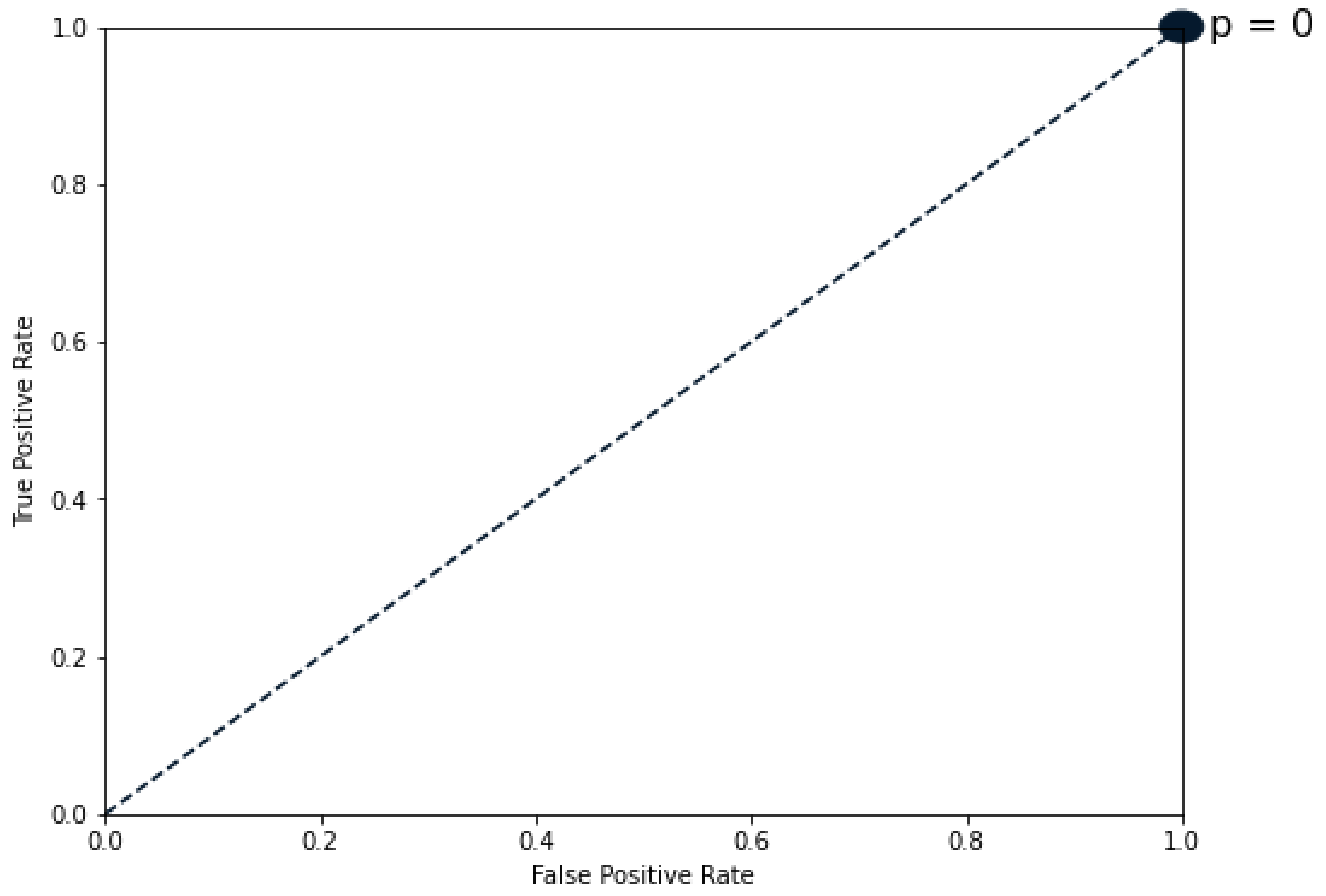
Probability thresholds

- By default, logistic regression threshold = 0.5
- Not specific to logistic regression
    - KNN classifiers also have thresholds
- What happens if we vary the threshold?

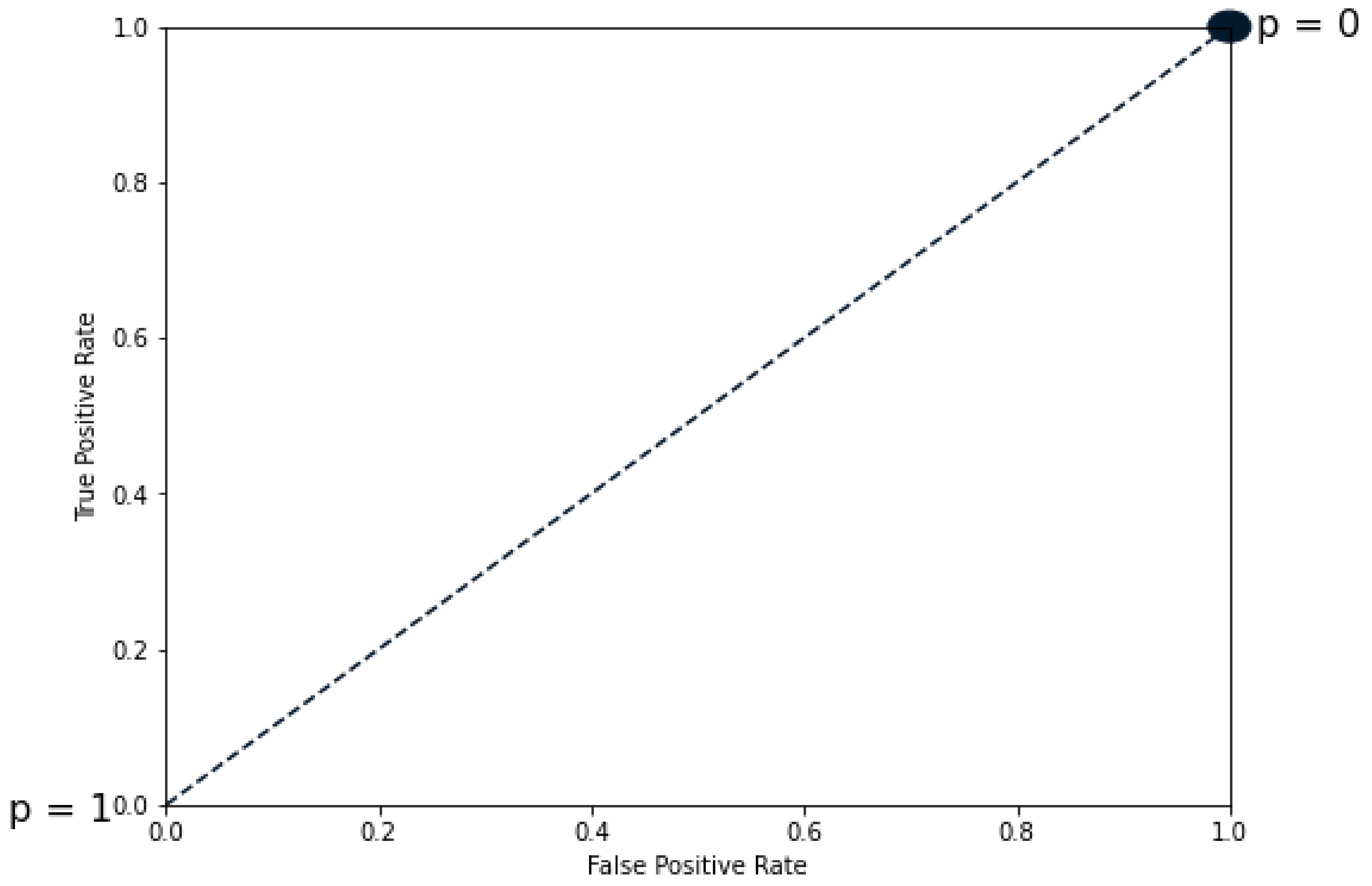
The ROC curve



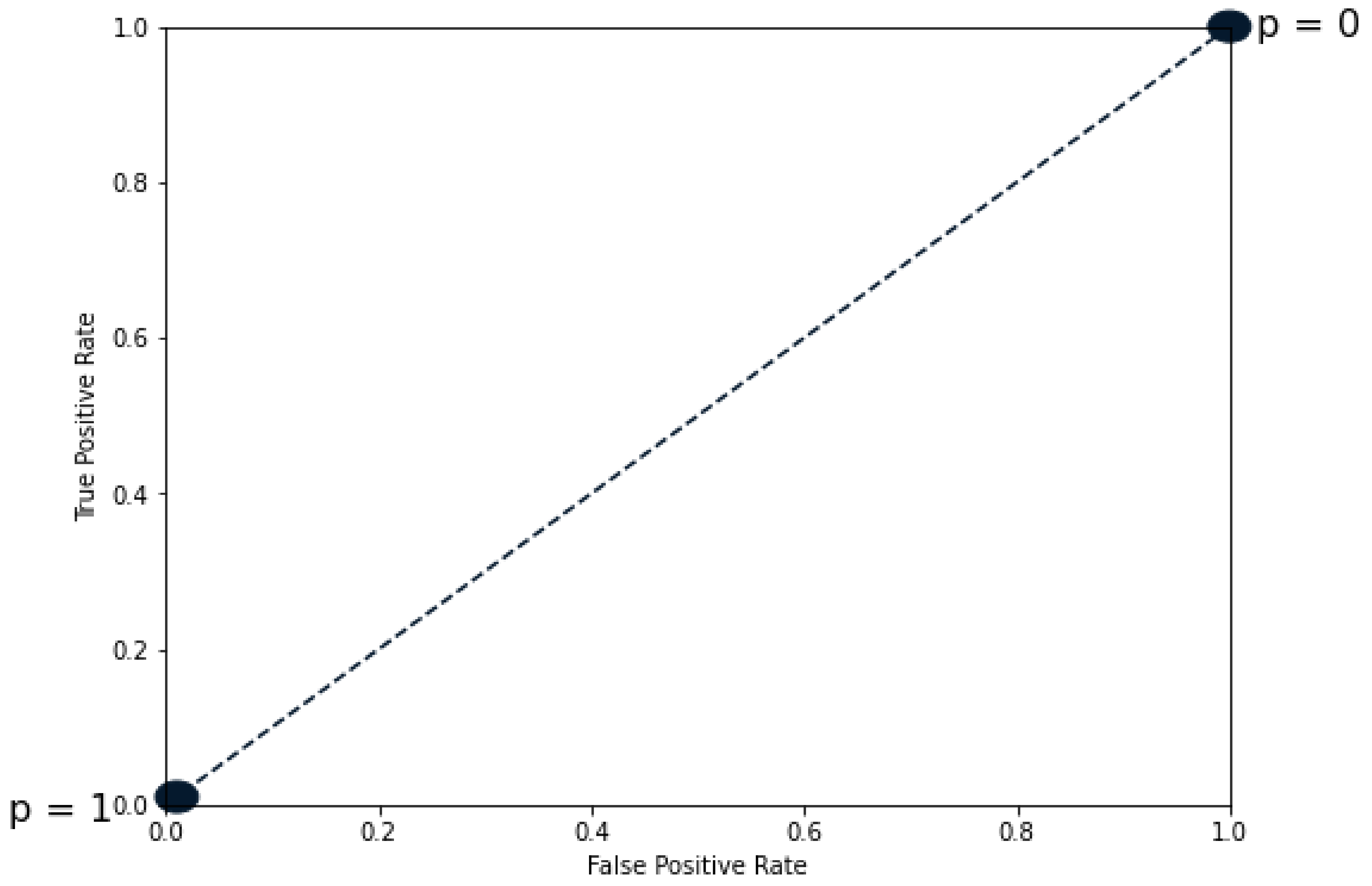
The ROC curve



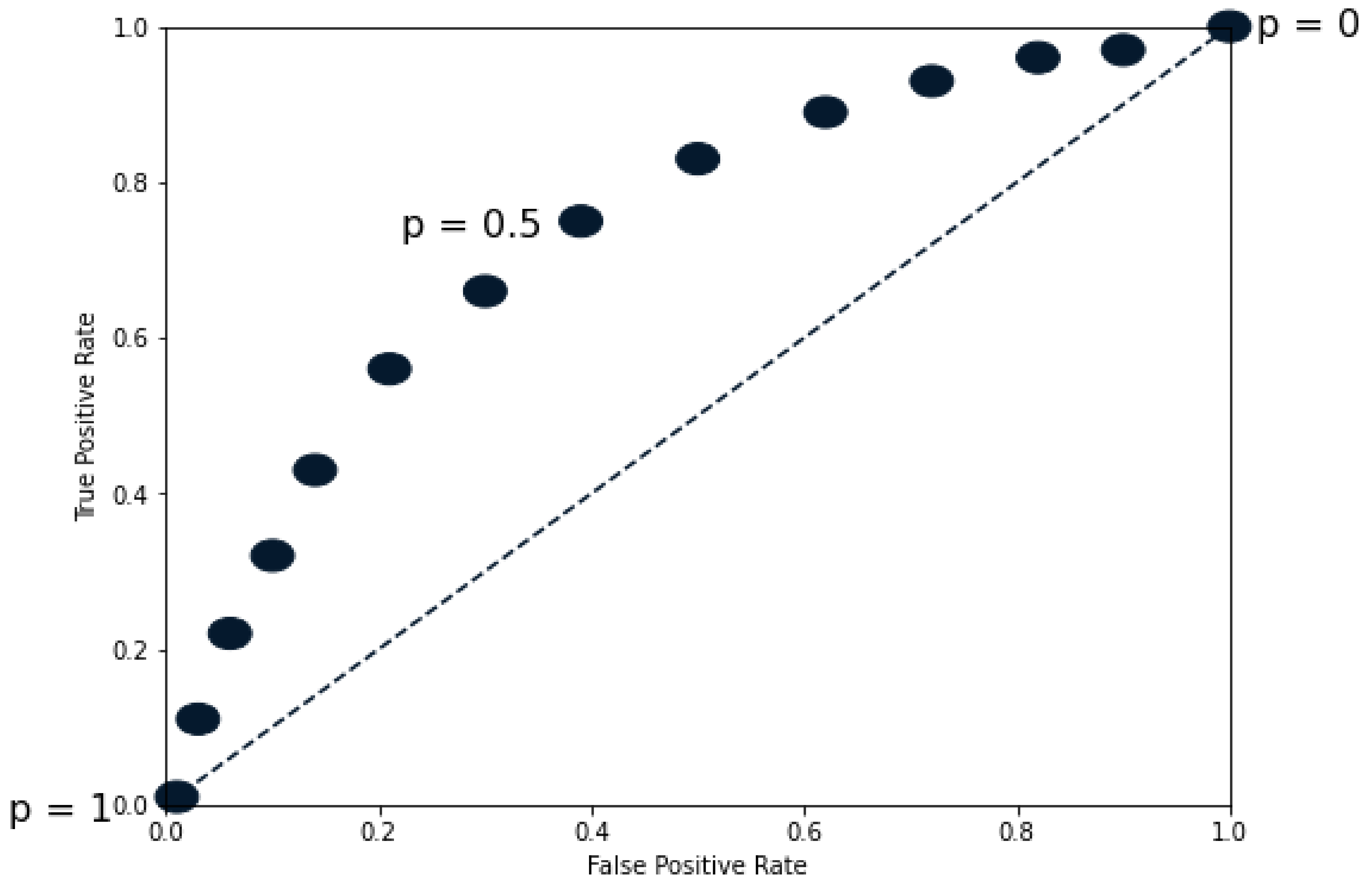
The ROC curve



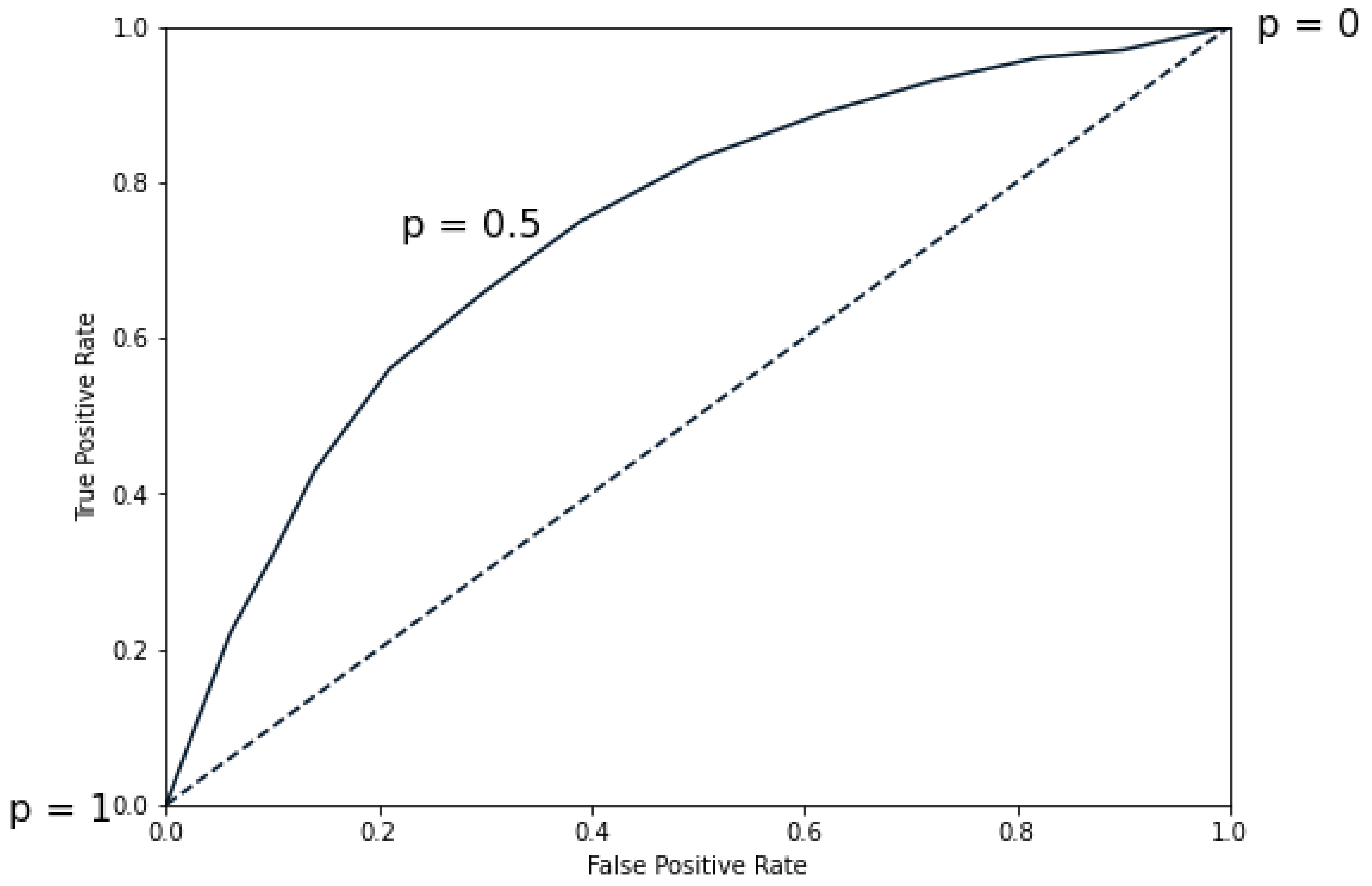
The ROC curve



The ROC curve



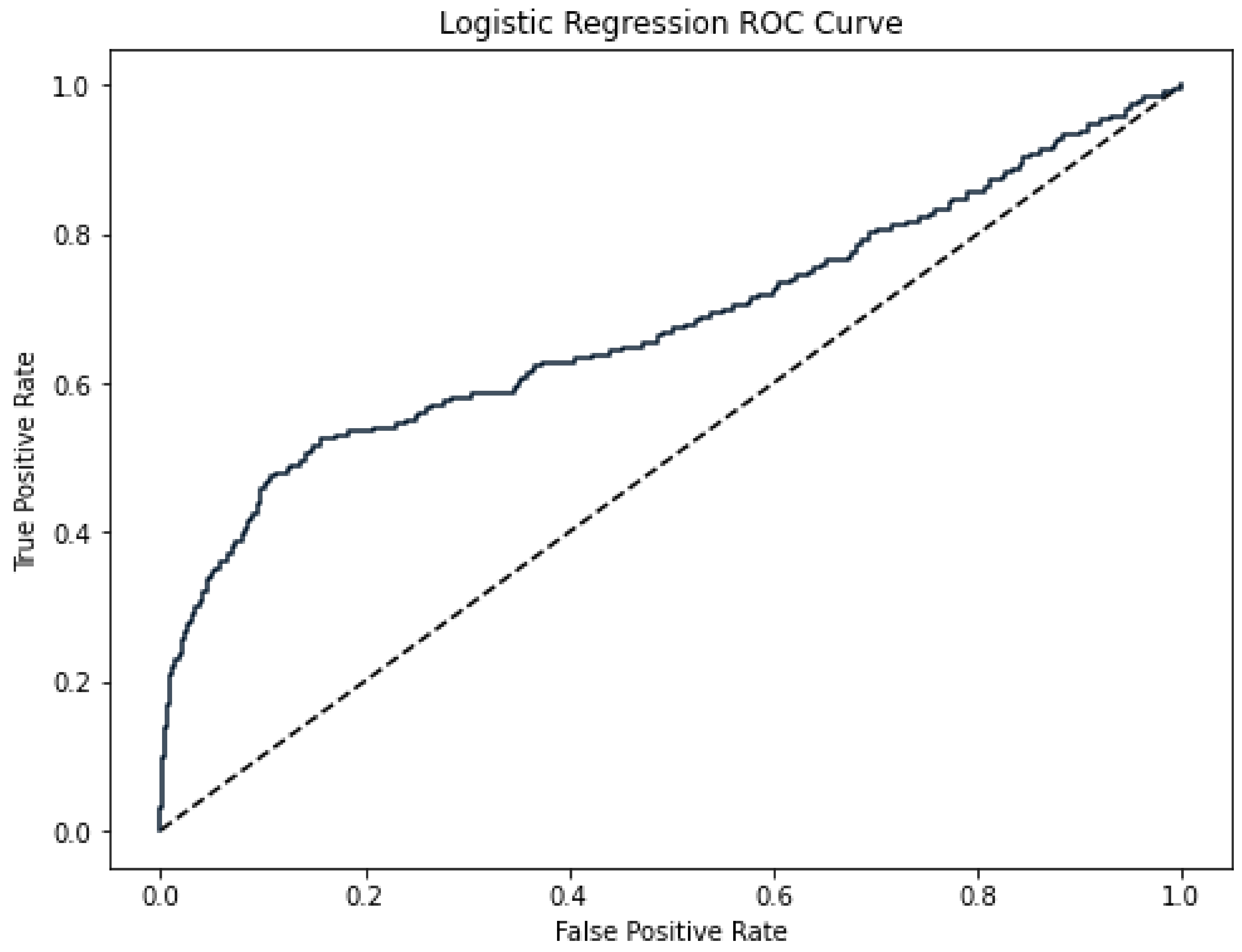
The ROC curve



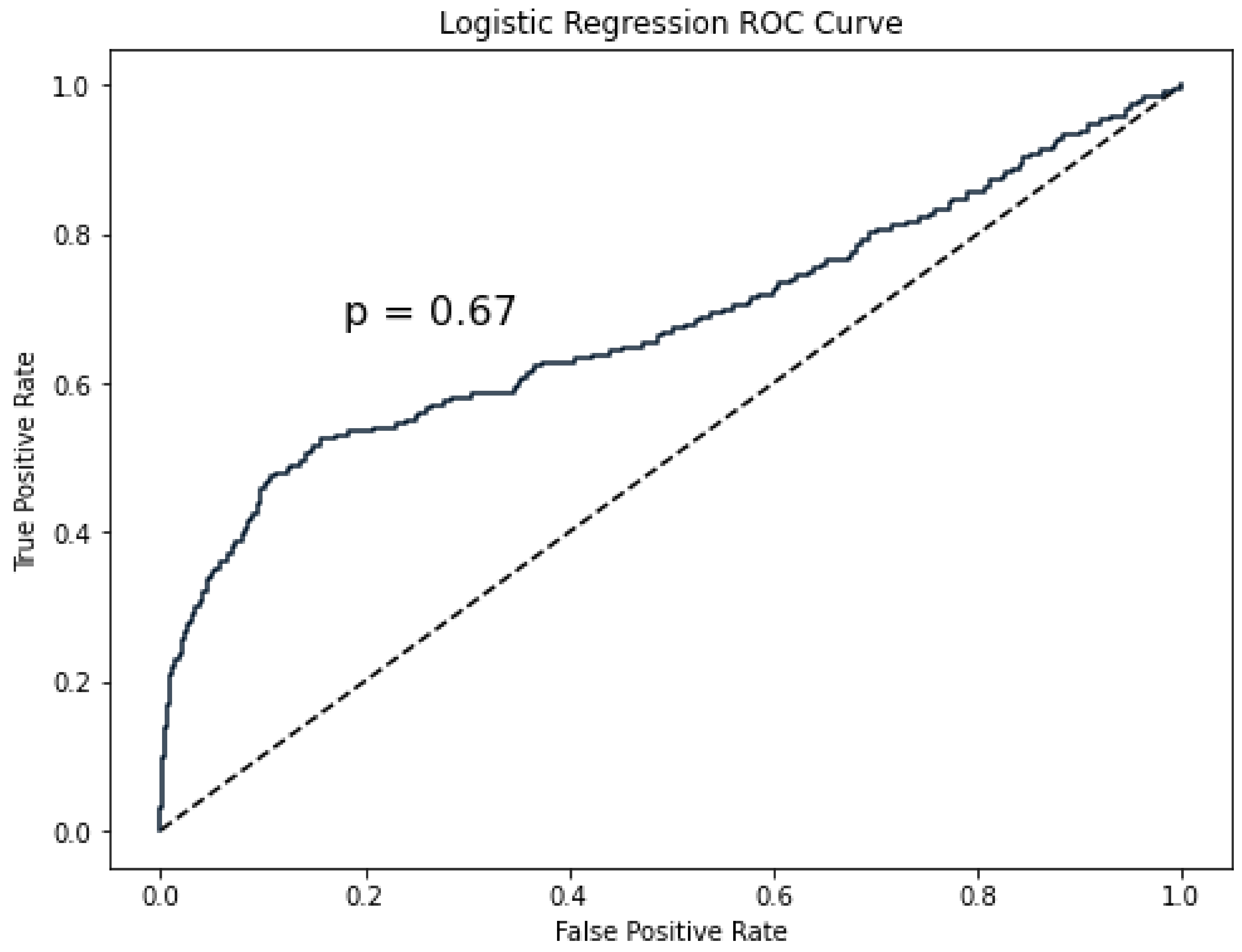
Plotting the ROC curve

```
from sklearn.metrics import roc_curve
fpr, tpr, thresholds = roc_curve(y_test, y_pred_probs)
plt.plot([0, 1], [0, 1], 'k--')
plt.plot(fpr, tpr)
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Logistic Regression ROC Curve')
plt.show()
```

Plotting the ROC curve



ROC AUC


Logistic Regression ROC Curve
p = 0.67
True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0

ROC AUC in scikit-learn

```python
from sklearn.metrics import roc_auc_score
print(roc_auc_score(y_test, y_pred_probs))
```

```
0.6700964152663693
```

Hyperparameter tuning

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Hyperparameter tuning

- Ridge/lasso regression: Choosing `alpha`
- KNN: Choosing `n_neighbors`
- Hyperparameters: Parameters we specify before fitting the model
    - Like `alpha` and `n_neighbors`

Choosing the correct hyperparameters

1. Try lots of different hyperparameter values
2. Fit all of them separately
3. See how well they perform
4. Choose the best performing values

- This is called **hyperparameter tuning**
- It is essential to use cross-validation to avoid overfitting to the test set
- We can still split the data and perform cross-validation on the training set
- We withhold the test set for final evaluation

Grid search cross-validation

	11		
	8		
	5		
n_neighbors	2		
		euclidean	manhattan
		metric	

Grid search cross-validation

	11	0.8716	0.8692
	8	0.8704	0.8688
	5	0.8748	0.8714
n_neighbors	2	0.8634	0.8646
		euclidean	manhattan
		metric	

Grid search cross-validation

	11	0.8716	0.8692
	8	0.8704	0.8688
	5	0.8748	0.8714
n_neighbors	2	0.8634	0.8646
		euclidean	manhattan
		metric	

GridSearchCV in scikit-learn

```python
from sklearn.model_selection import GridSearchCV
kf = KFold(n_splits=5, shuffle=True, random_state=42)
param_grid = {"alpha": np.arange(0.0001, 1, 10),
              "solver": ["sag", "lsqr"]}
ridge = Ridge()
ridge_cv = GridSearchCV(ridge, param_grid, cv=kf)
ridge_cv.fit(X_train, y_train)
print(ridge_cv.best_params_, ridge_cv.best_score_)
```

```
{'alpha': 0.0001, 'solver': 'sag'}
0.7529912278705785
```

Limitations and an alternative approach

- 3-fold cross-validation, 1 hyperparameter, 10 total values = 30 fits
- 10 fold cross-validation, 3 hyperparameters, 30 total values = 900 fits

RandomizedSearchCV

```python
from sklearn.model_selection import RandomizedSearchCV
kf = KFold(n_splits=5, shuffle=True, random_state=42)
param_grid = {'alpha': np.arange(0.0001, 1, 10),
              "solver": ['sag', 'lsqr']}
ridge = Ridge()
ridge_cv = RandomizedSearchCV(ridge, param_grid, cv=kf, n_iter=2)
ridge_cv.fit(X_train, y_train)
print(ridge_cv.best_params_, ridge_cv.best_score_)
```

```
{'solver': 'sag', 'alpha': 0.0001}
0.7529912278705785
```

Evaluating on the test set

```python
test_score = ridge_cv.score(X_test, y_test)
print(test_score)
```

```
0.7564731534089224
```