How good is your model?

SUPERVISED LEARNING WITH SCIKIT-LEARN

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Classification metrics

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

Class imbalance example: Emails

- Spam classification
  - 99% of emails are real; 1% of emails are spam
- Could build a classifier that predicts ALL emails as real
  - 99% accurate!
  - But horrible at actually classifying spam
  - Fails at its original purpose
- Need more nuanced metrics

Diagnosing classification predictions

- Confusion matrix

	Predicted: Spam Email	Predicted: Real Email
Actual: Spam Email	True Positive	False Negative
Actual: Real Email	False Positive	True Negative

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- Accuracy:

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

Metrics from the confusion matrix

- Precision $\frac{tp}{tp+fp}$
- Recall $\frac{tp}{tp+fn}$
- F1score: $2 \cdot \frac{precision * recall}{precision + recall}$
- High precision: Not many real emails predicted as spam
- High recall: Predicted most spam emails correctly

Confusion matrix in scikit-learn

```
from sklearn.metrics import classification_report
from sklearn.metrics import confusion_matrix
knn = KNeighborsClassifier(n_neighbors=8)
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))
```

```
[[52  7]
 [ 3 112]]
```

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

```
             precision    recall  f1-score   support
          0       0.95      0.88      0.91        59
          1       0.94      0.97      0.96       115
avg / total       0.94      0.94      0.94       174
```

Let's practice!

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Logistic regression and the ROC curve

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Logistic regression for binary classification

- Logistic regression outputs probabilities
- If the probability ‘p’ is greater than 0.5:
  - The data is labeled ‘1’
- If the probability ‘p’ is less than 0.5:
- The data is labeled ‘0’

Linear decision boundary

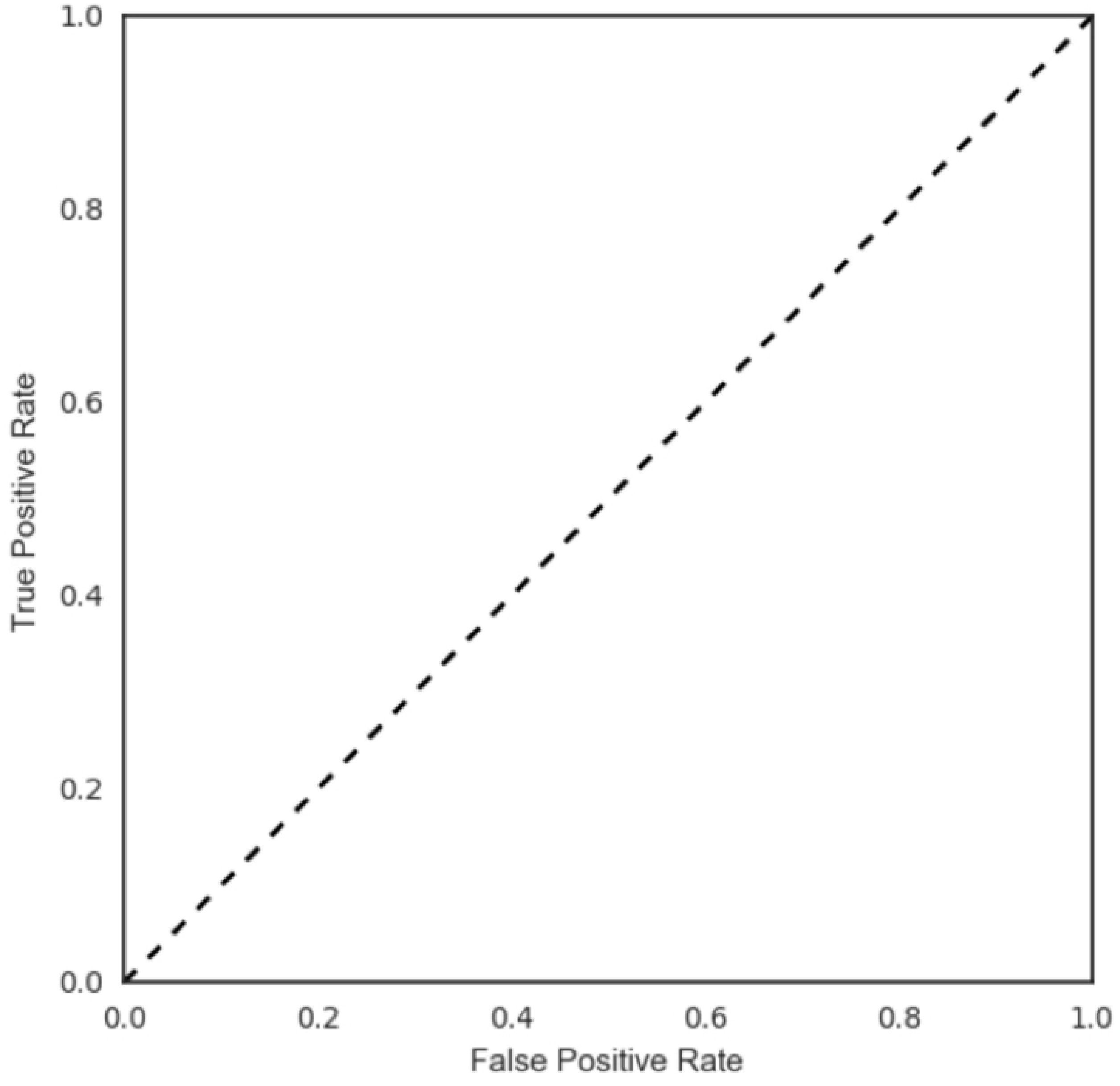
Logistic regression in scikit-learn

```
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split
logreg = LogisticRegression()
X_train, X_test, y_train, y_test = train_test_split(X, y,
    test_size=0.4, random_state=42)
logreg.fit(X_train, y_train)
y_pred = logreg.predict(X_test)
```

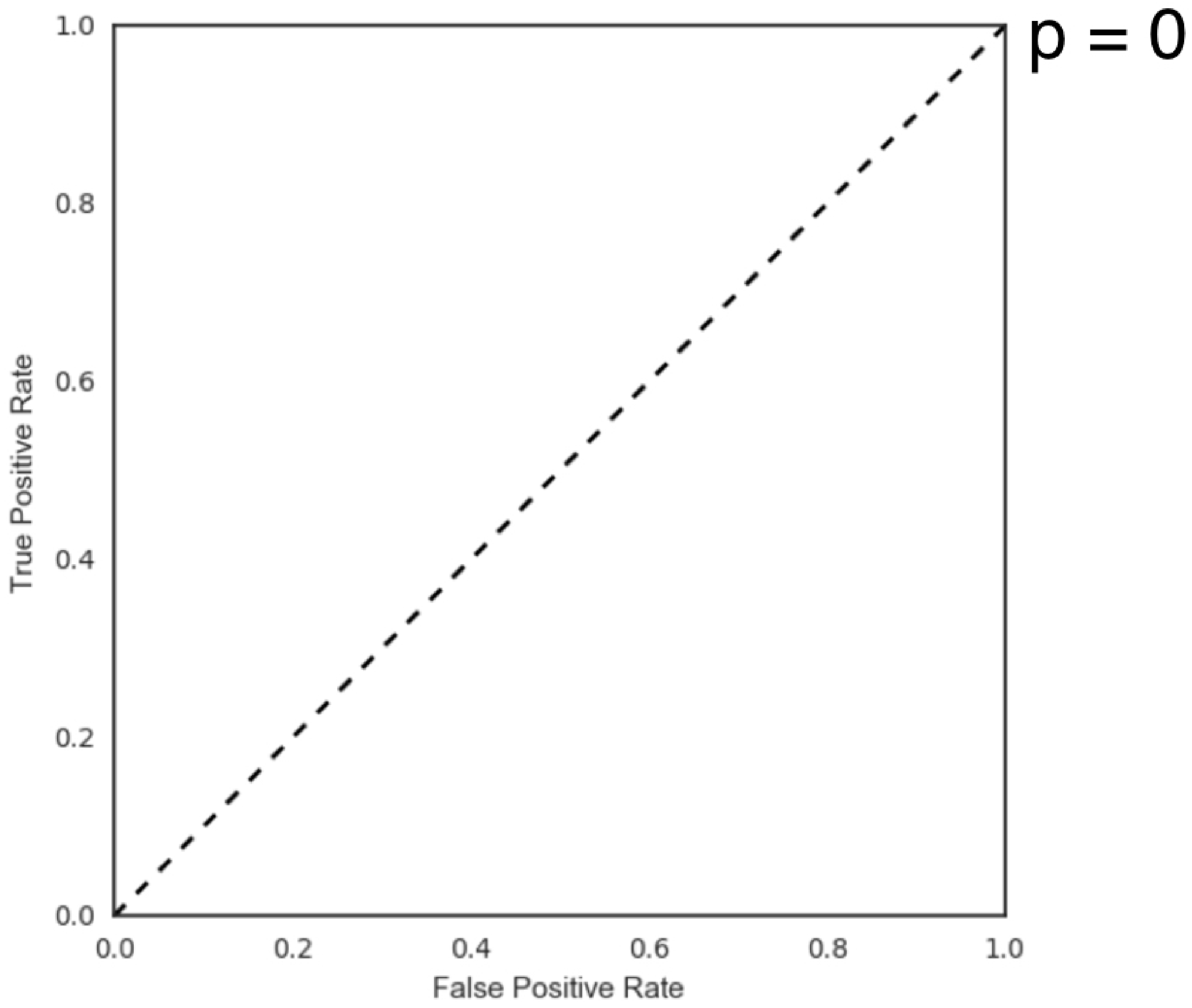
Probability thresholds

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

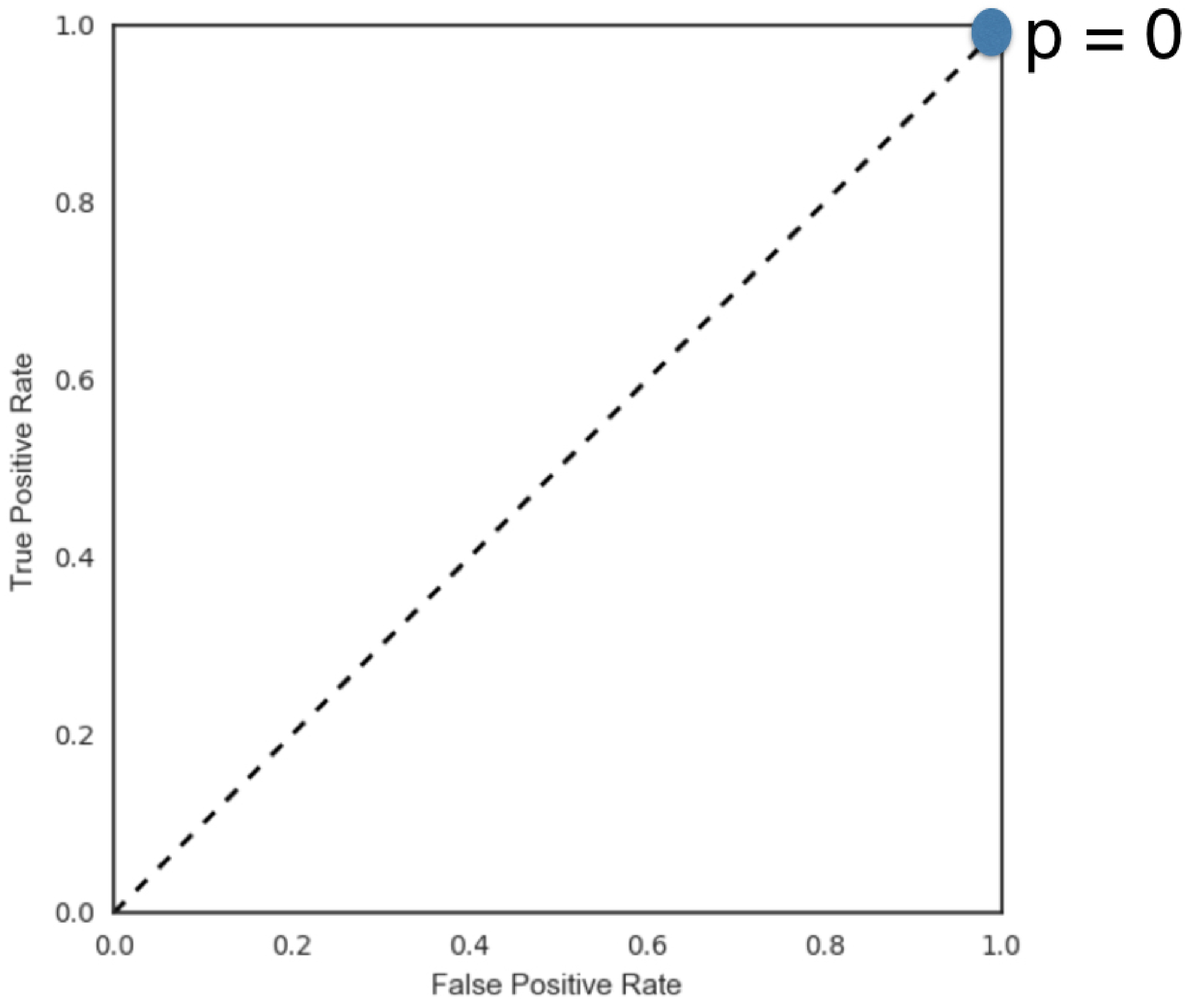
The ROC curve



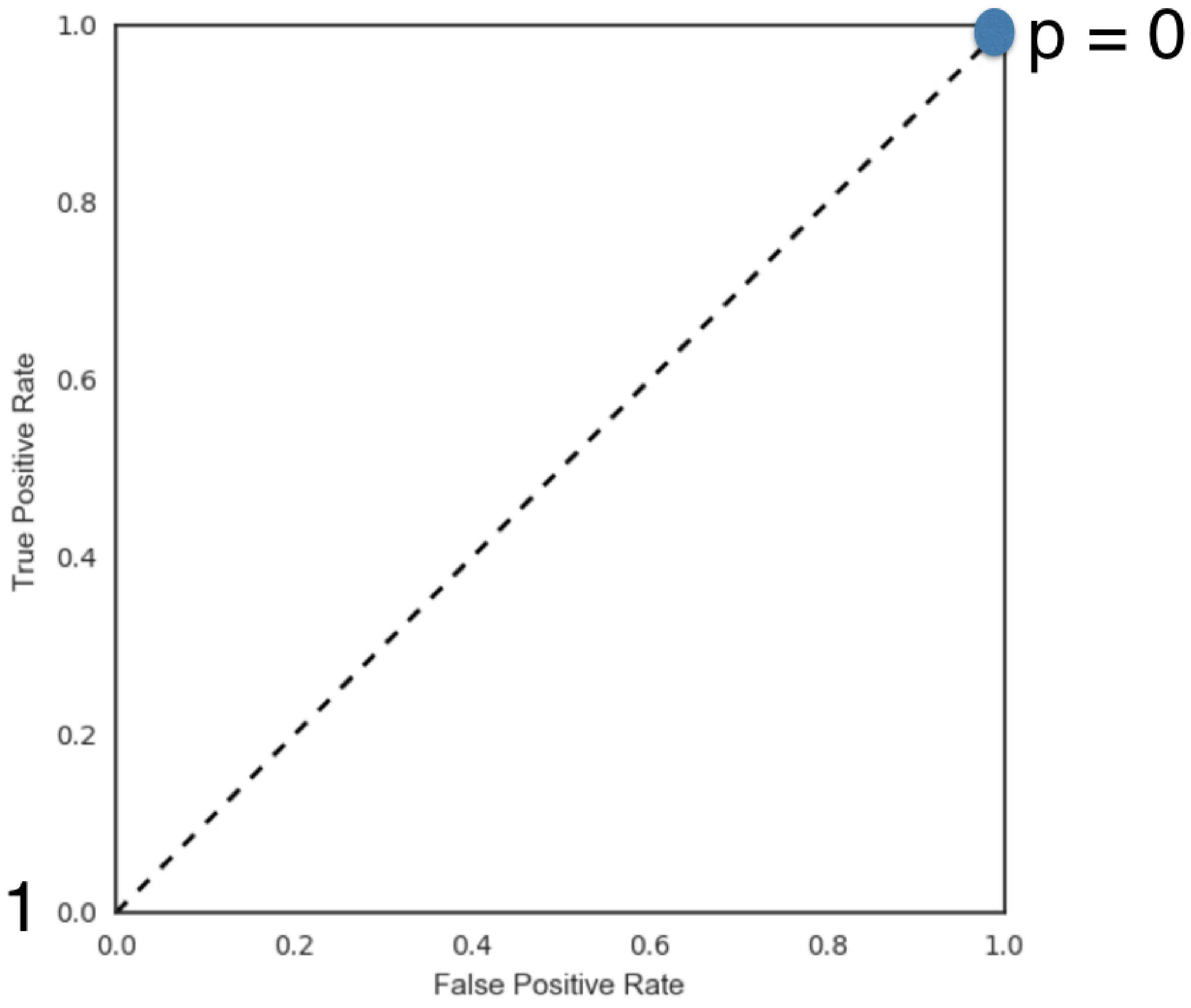
The ROC curve



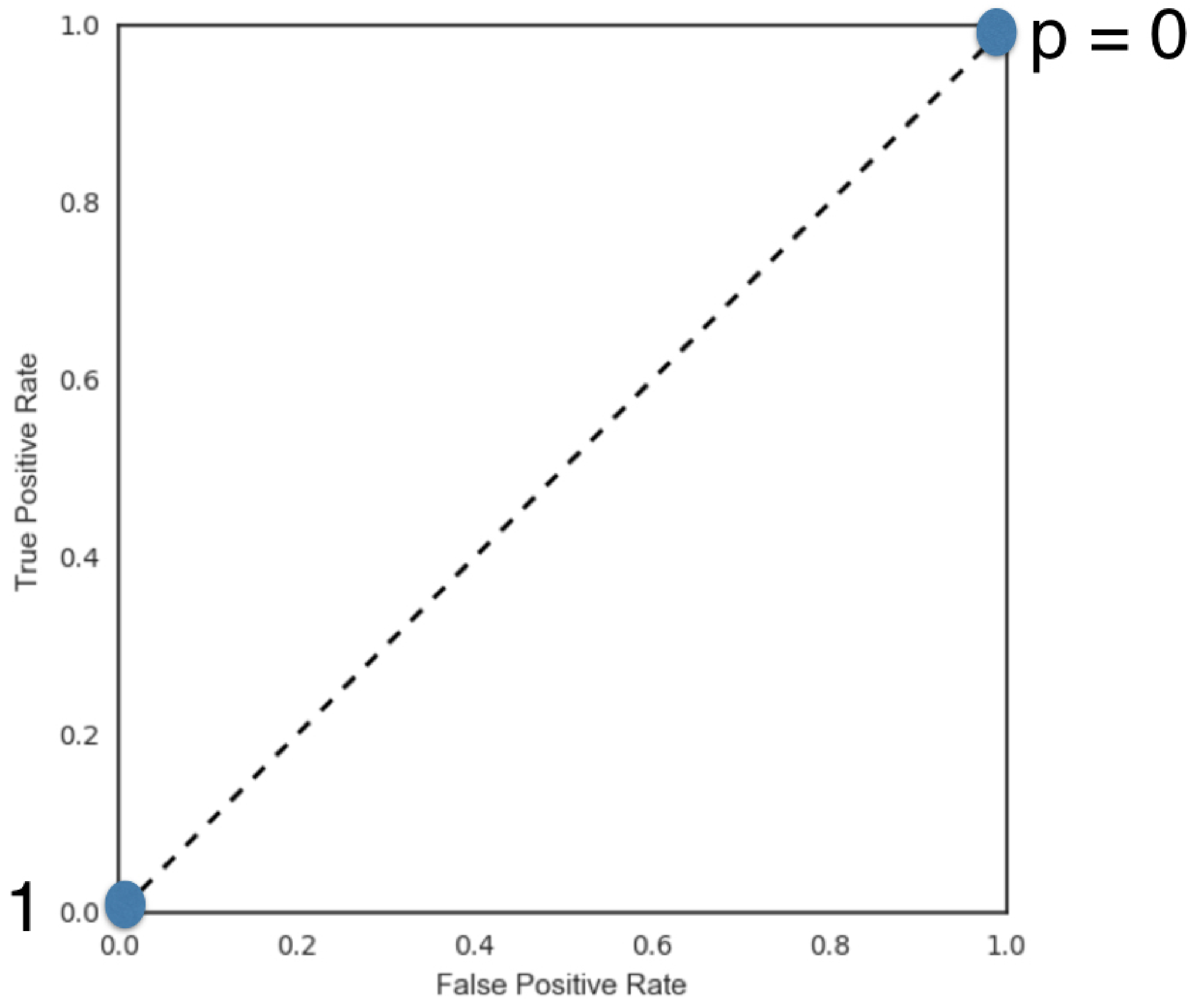
The ROC curve



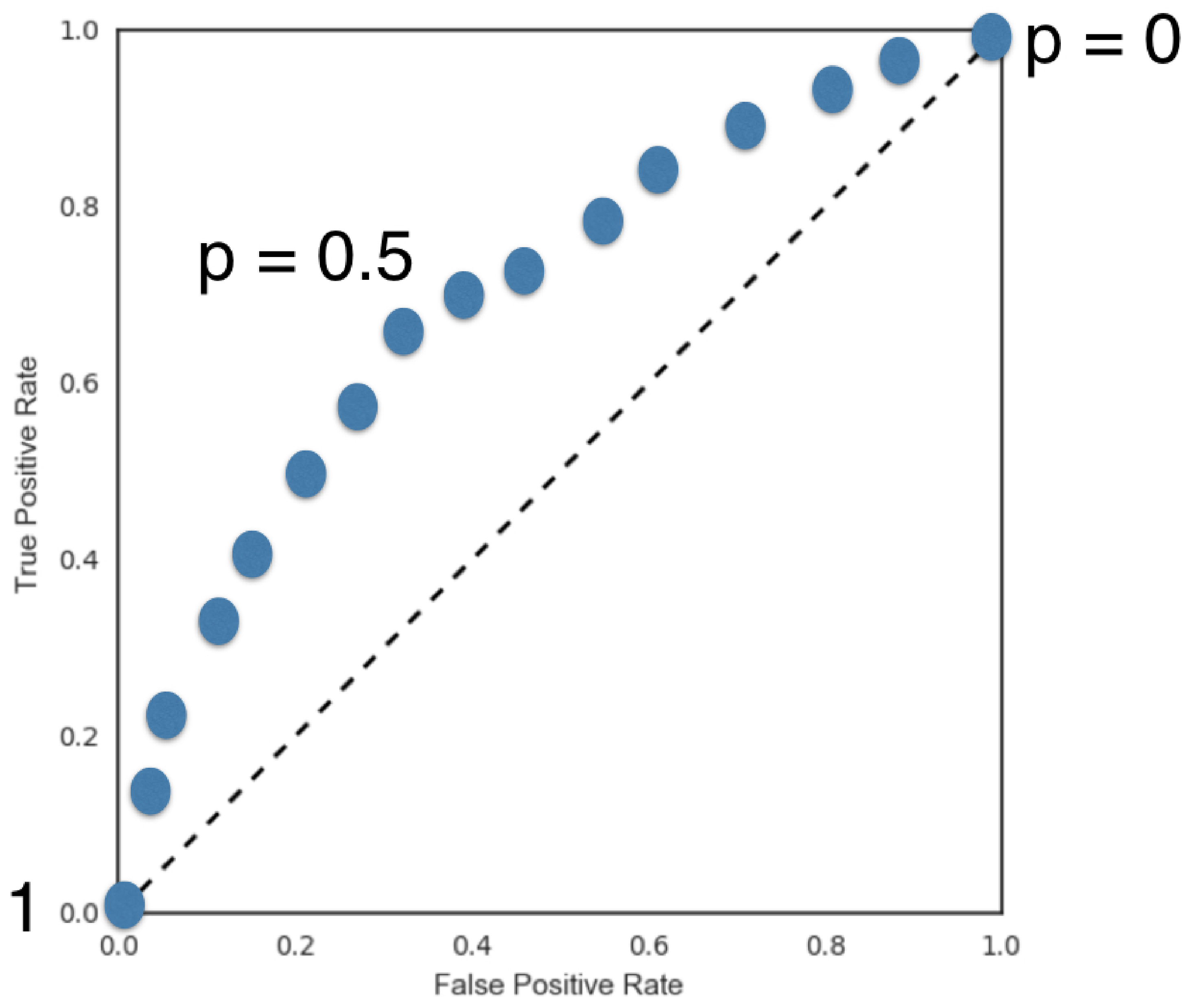
The ROC curve



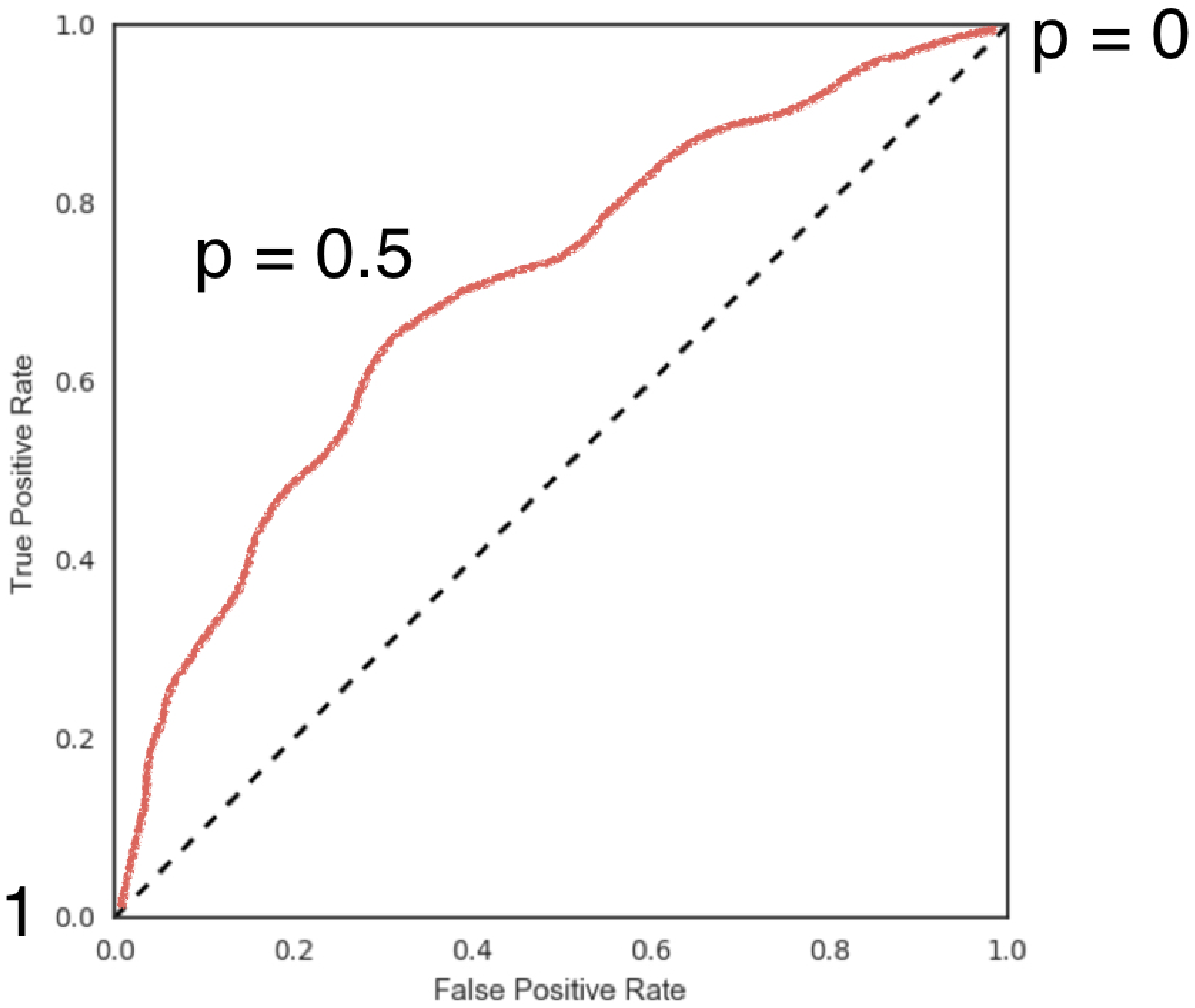
The ROC curve



The ROC curve



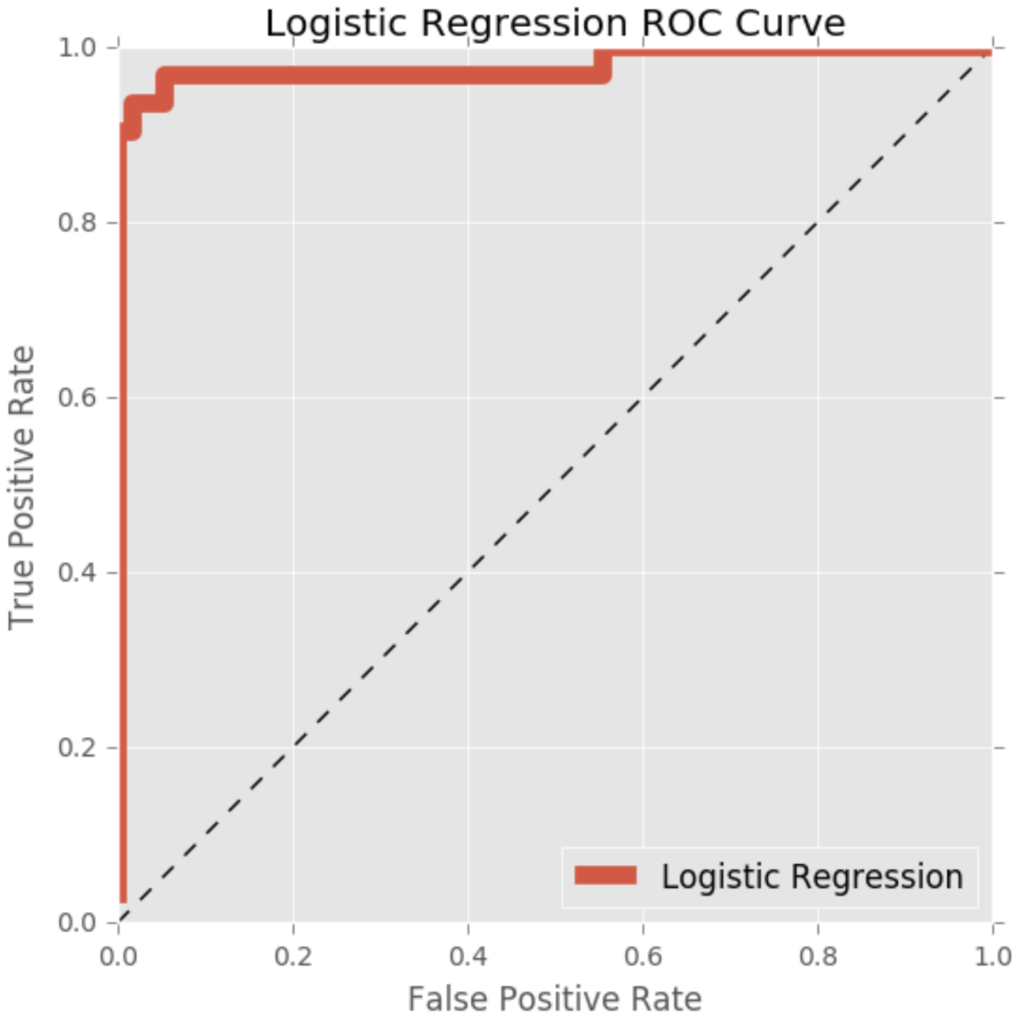
The ROC curve



Plotting the ROC curve

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

Plotting the ROC curve




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

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Area under the ROC curve

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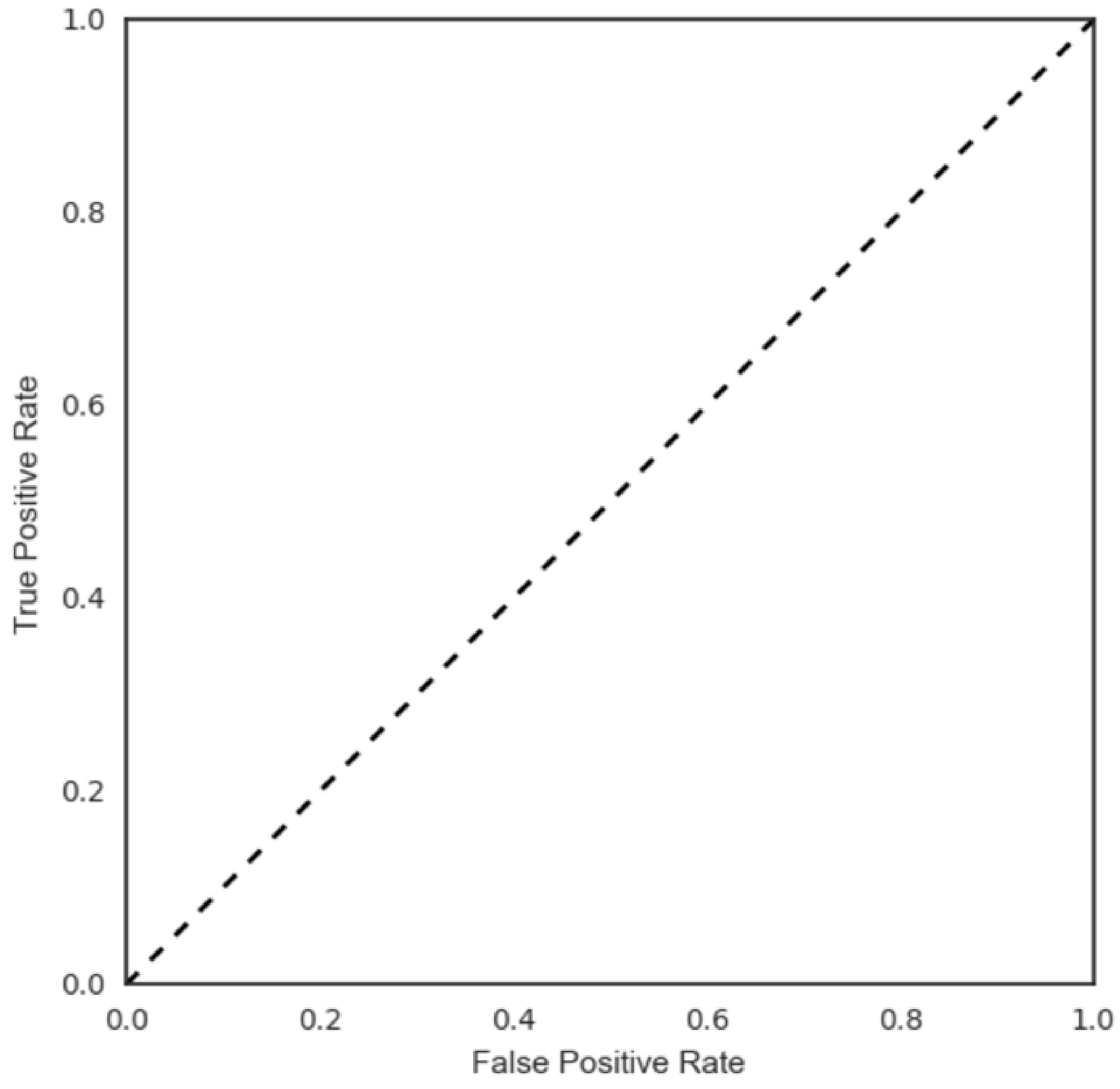
Area under the ROC curve (AUC)

- Larger area under the ROC curve = better model



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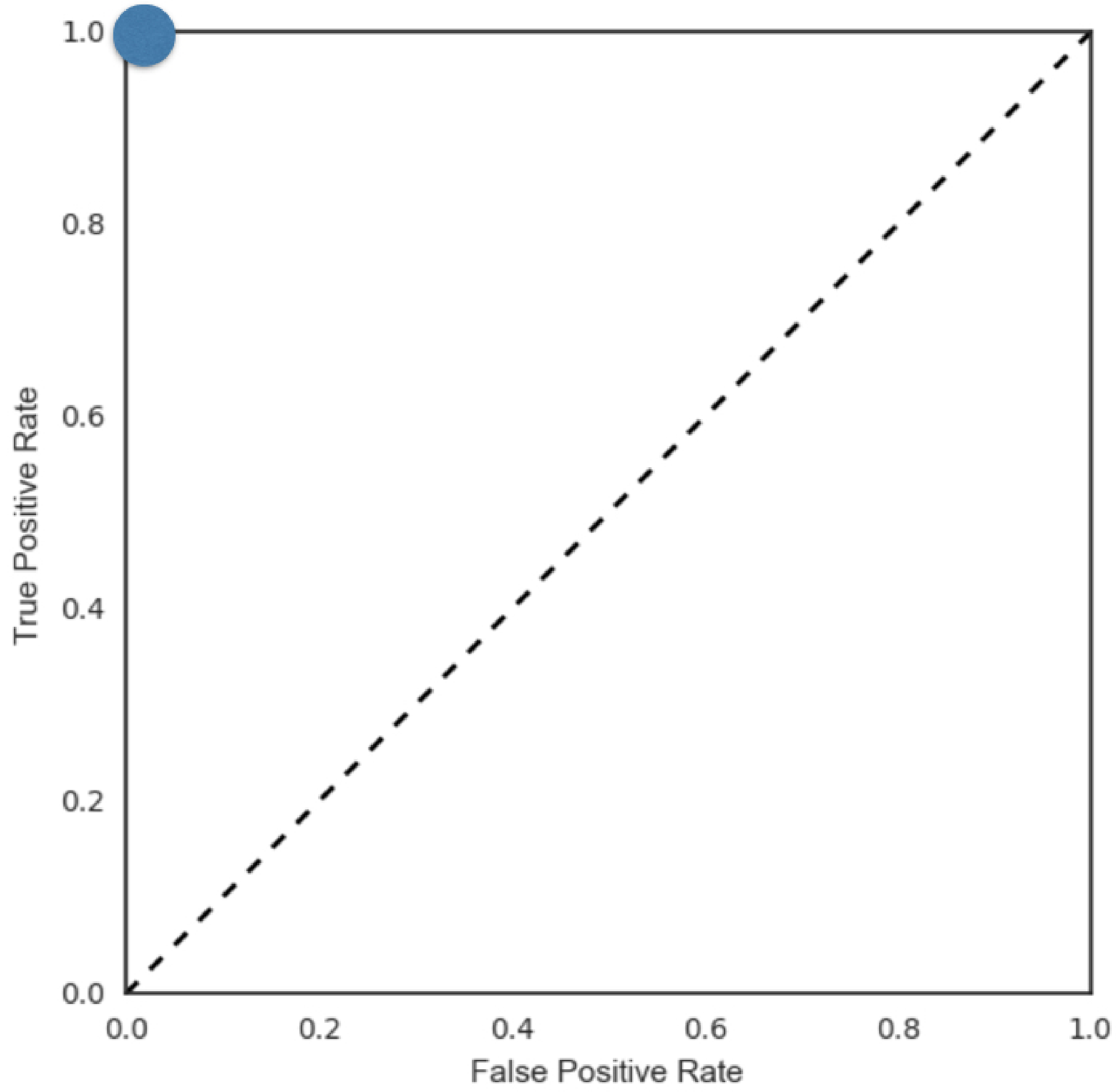

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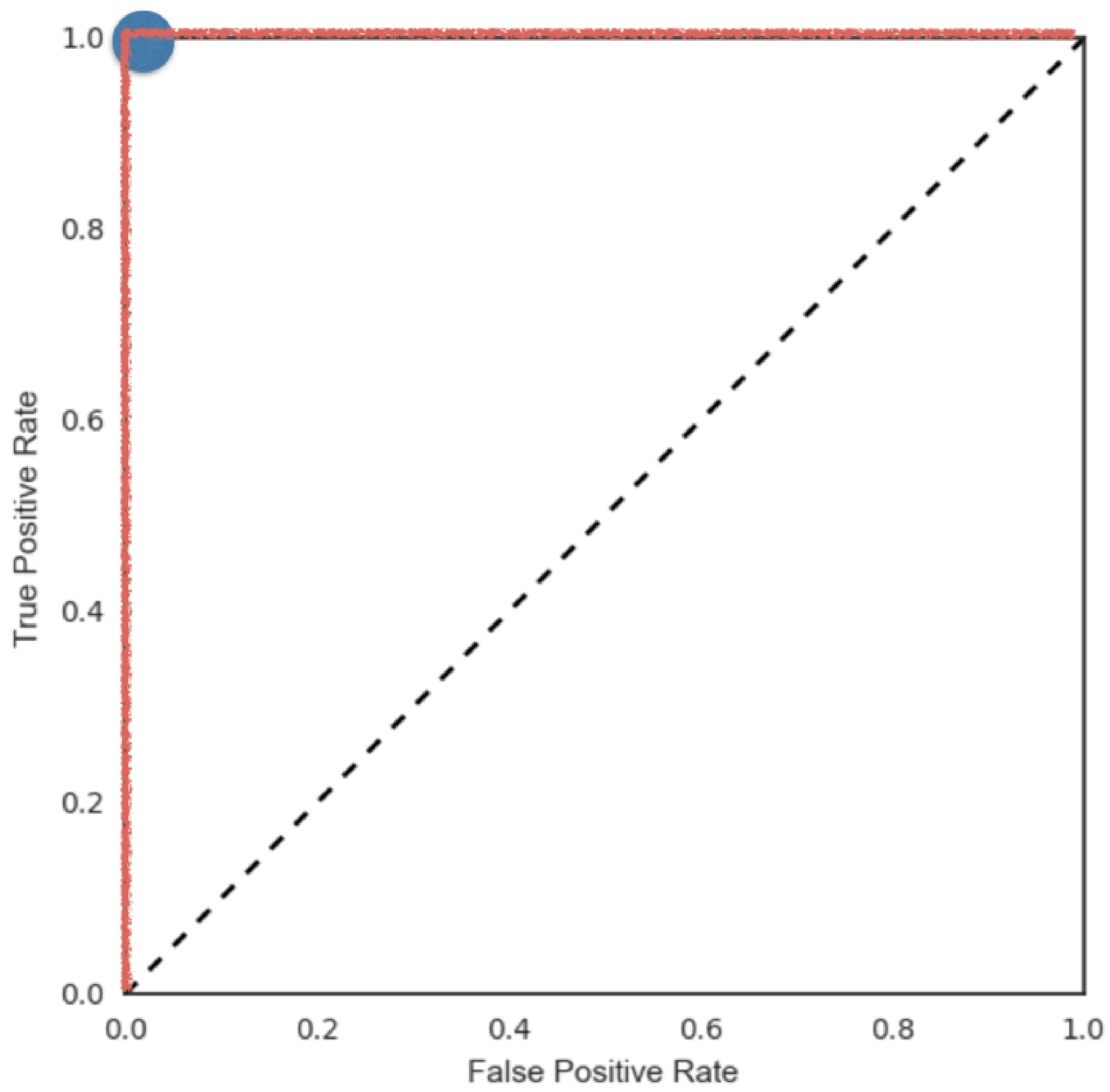

Area under the ROC curve (AUC)

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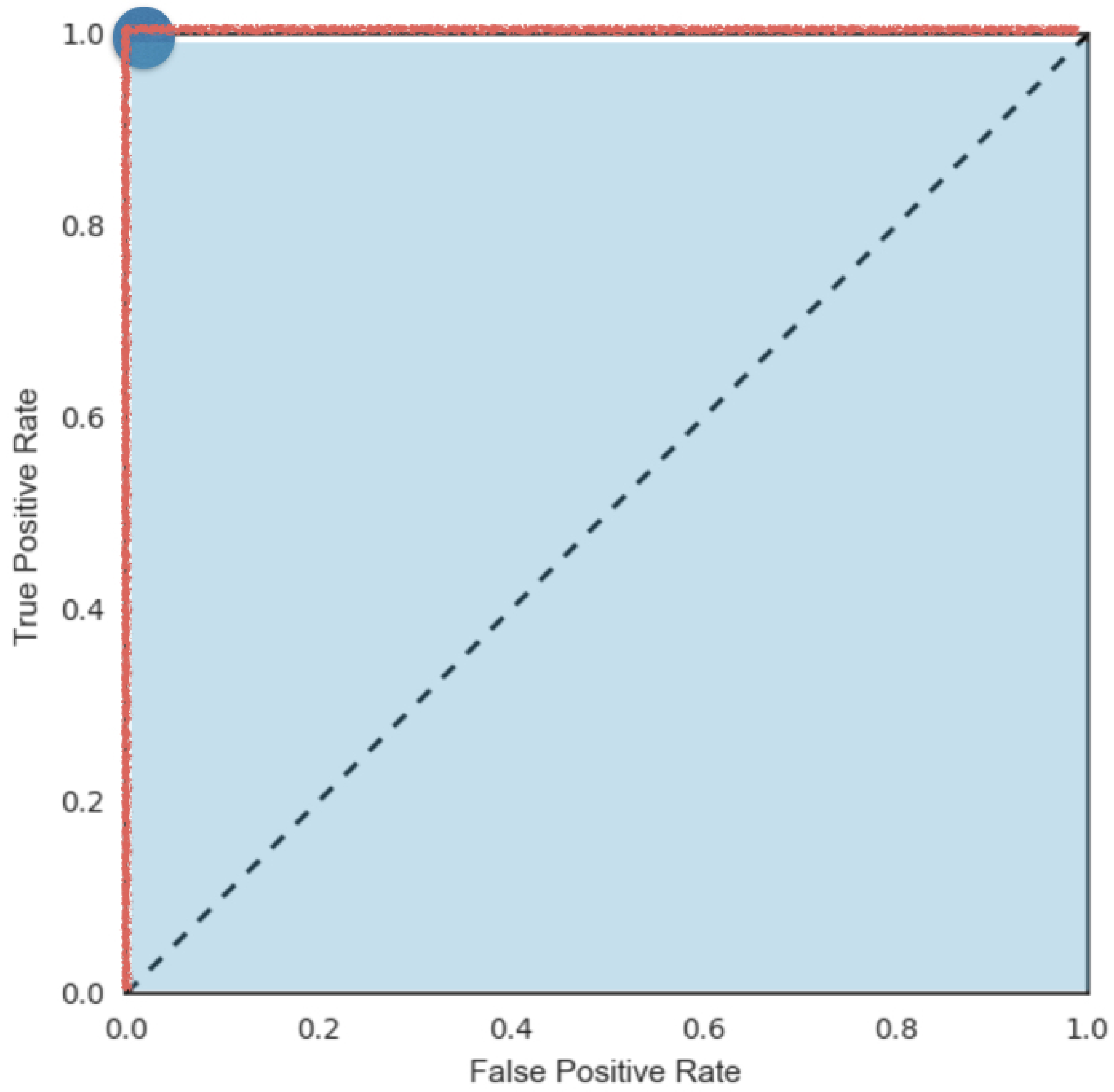

AUC in scikit-learn

```python
from sklearn.metrics import roc_auc_score
logreg = LogisticRegression()
X_train, X_test, y_train, y_test = train_test_split(X, y,
    test_size=0.4, random_state=42)
logreg.fit(X_train, y_train)
y_pred_prob = logreg.predict_proba(X_test)[:,1]
roc_auc_score(y_test, y_pred_prob)
```

```
0.997466216216
```

AUC using cross-validation

```python
from sklearn.model_selection import cross_val_score
cv_scores = cross_val_score(logreg, X, y, cv=5,
                            scoring='roc_auc')
print(cv_scores)
```

```
[ 0.99673203  0.99183007  0.99583796  1.          0.96140652]
```

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Hyperparameter tuning

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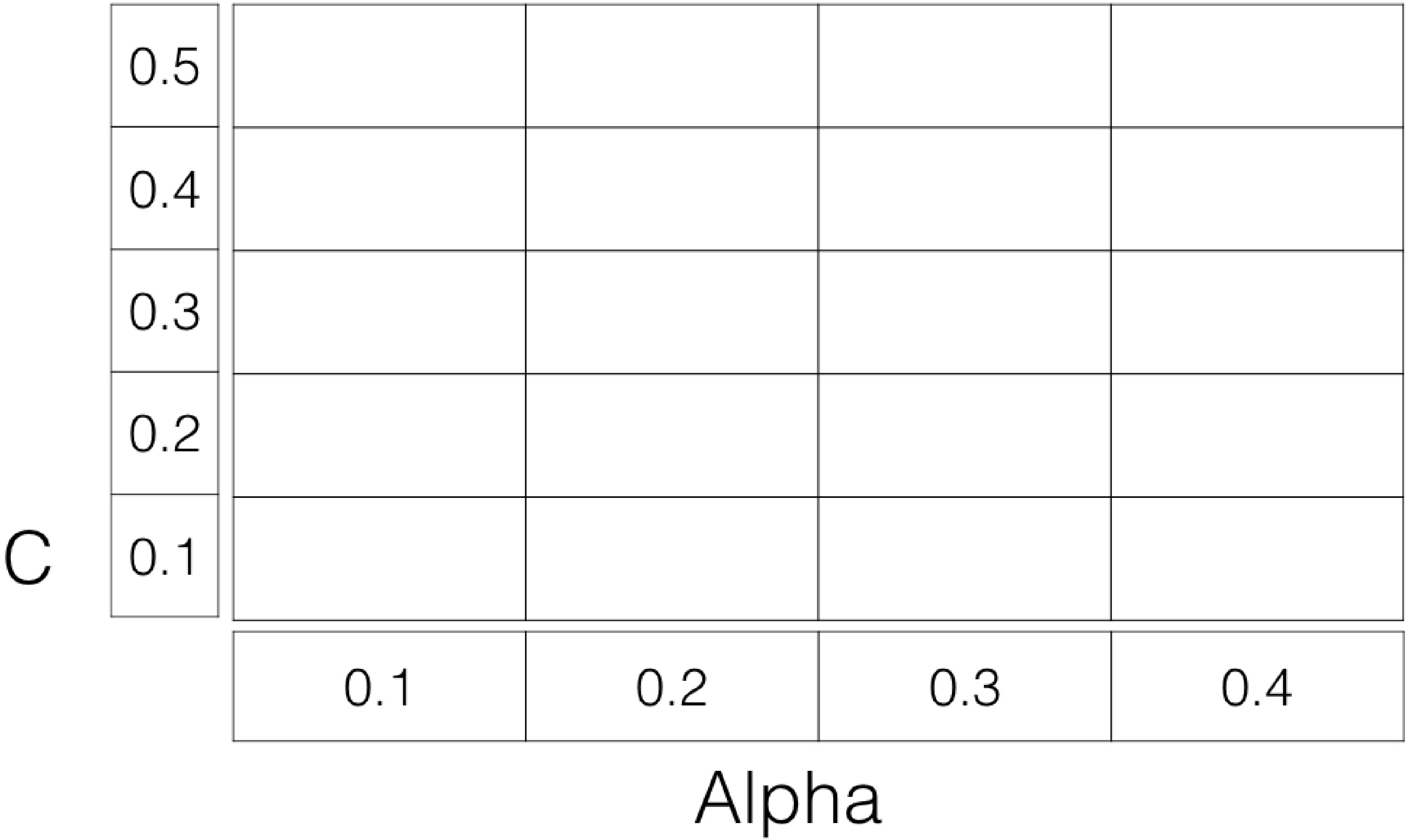
Hyperparameter tuning

- Linear regression: Choosing parameters
- Ridge/lasso regression: Choosing alpha
- k-Nearest Neighbors: Choosing n_neighbors
- Parameters like alpha and k: Hyperparameters
- Hyperparameters cannot be learned by fitting the model

Choosing the correct hyperparameter

- Try a bunch of different hyperparameter values
- Fit all of them separately
- See how well each performs
- Choose the best performing one
- It is essential to use cross-validation

Grid search cross-validation



Grid search cross-validation

C \ Alpha	0.1	0.2	0.3	0.4
0.5	0.701	0.703	0.697	0.696
0.4	0.699	0.702	0.698	0.702
0.3	0.721	0.726	0.713	0.703
0.2	0.706	0.705	0.704	0.701
0.1	0.698	0.692	0.688	0.675

Grid search cross-validation

C				
0.5	0.701	0.703	0.697	0.696
0.4	0.699	0.702	0.698	0.702
0.3	0.721	0.726	0.713	0.703
0.2	0.706	0.705	0.704	0.701
0.1	0.698	0.692	0.688	0.675
	0.1	0.2	0.3	0.4
		Alpha		

GridSearchCV in scikit-learn

```
from sklearn.model_selection import GridSearchCV
param_grid = {'n_neighbors': np.arange(1, 50)}
knn = KNeighborsClassifier()
knn_cv = GridSearchCV(knn, param_grid, cv=5)
knn_cv.fit(X, y)
knn_cv.best_params_
```

```
{'n_neighbors': 12}
```

```
knn_cv.best_score_
```

```
0.933216168717
```

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Hold-out set for final evaluation

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Hold-out set reasoning

- How well can the model perform on never before seen data?
- Using ALL data for cross-validation is not ideal
- Split data into training and hold-out set at the beginning
- Perform grid search cross-validation on training set
- Choose best hyperparameters and evaluate on hold-out set

Let's practice!

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