01_machine_learning_workflow

September 29, 2021

1 Basic Walk-Through: k-nearest Neighbors

This notebook contains several examples that illustrate the machine learning workflow using a dataset of house prices.

We will use the fairly straightforward k-nearest neighbors (KNN) algorithm that allows us to tackle both regression and classification problems.

In its default sklearn implementation, it identifies the k nearest data points (based on the Euclidean distance) to make a prediction. It predicts the most frequent class among the neighbors or the average outcome in the classification or regression case, respectively.

[1]:
```
import warnings
from pathlib import Path
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
from scipy.stats import spearmanr
from sklearn.neighbors import KNeighborsClassifier, KNeighborsRegressor
from sklearn.model_selection import cross_val_score, cross_val_predict,␣
↪validation_curve, learning_curve, GridSearchCV
from sklearn.feature_selection import mutual_info_regression,␣
↪mutual_info_classif
from sklearn.preprocessing import StandardScaler, scale
from sklearn.pipeline import Pipeline
from sklearn.metrics import make_scorer
from yellowbrick.model_selection import ValidationCurve, LearningCurve
```

[2]:
```
%matplotlib inline
plt.style.use('fivethirtyeight')
warnings.filterwarnings('ignore')
```

1.1 Get the Data

1.1.1 Kings County Housing Data

Data from Kaggle

Download via API:

```
kaggle datasets download -d harlfoxem/housesalesprediction
```

[3]:
```python
DATA_PATH = Path('..', 'data')
```

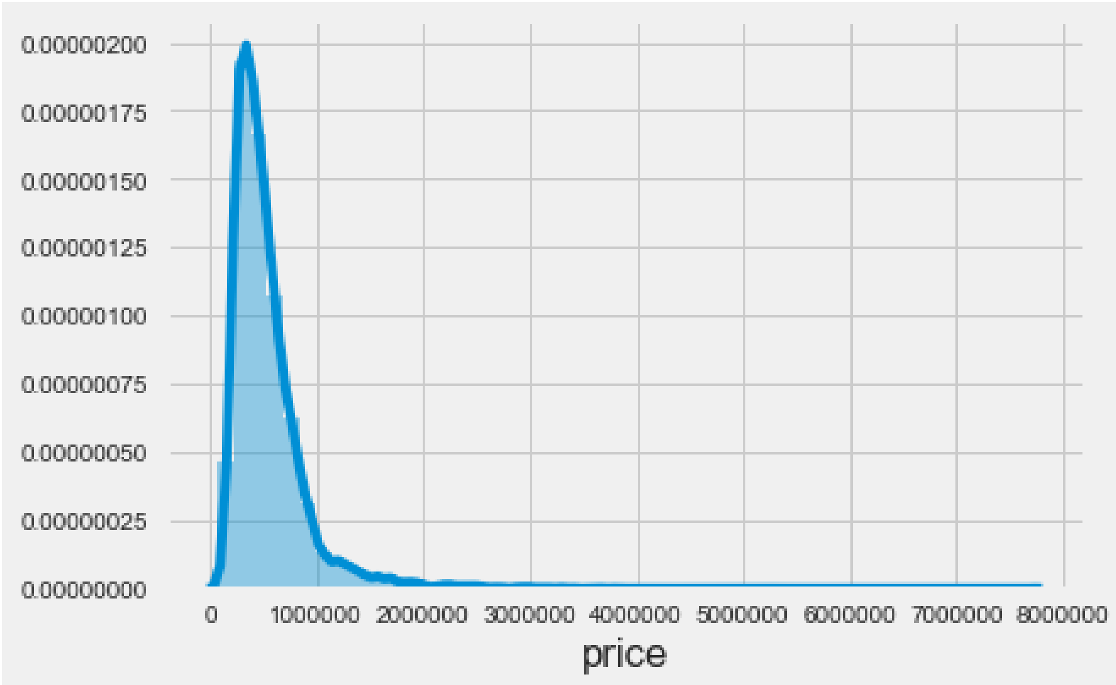
[4]:
```python
house_sales = pd.read_csv(DATA_PATH / 'kc_house_data.csv')
house_sales = house_sales.drop(
    ['id', 'zipcode', 'lat', 'long', 'date'], axis=1)
house_sales.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 21613 entries, 0 to 21612
Data columns (total 16 columns):
price            21613 non-null float64
bedrooms         21613 non-null int64
bathrooms        21613 non-null float64
sqft_living      21613 non-null int64
sqft_lot         21613 non-null int64
floors           21613 non-null float64
waterfront       21613 non-null int64
view             21613 non-null int64
condition        21613 non-null int64
grade            21613 non-null int64
sqft_above       21613 non-null int64
sqft_basement    21613 non-null int64
yr_built         21613 non-null int64
yr_renovated     21613 non-null int64
sqft_living15    21613 non-null int64
sqft_lot15       21613 non-null int64
dtypes: float64(3), int64(13)
memory usage: 2.6 MB
```

1.2 Select & Transform Features

1.2.1 Asset Prices often have long tails

[5]:
```python
sns.distplot(house_sales.price);
```



1.2.2 Use log-transform

Useful for dealing with skewed data.

[6]:
```
X_all = house_sales.drop('price', axis=1)
y = np.log(house_sales.price)
```

1.2.3 Mutual information regression

See sklearn docs. Covered later in Chapter 6 of the book.

[7]:
```
mi_reg = pd.Series(mutual_info_regression(X_all, y),
                   index=X_all.columns).sort_values(ascending=False)
mi_reg
```

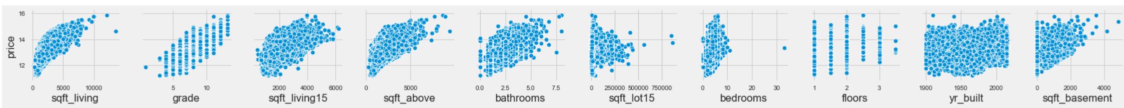
[7]:
```
sqft_living      0.347869
grade            0.344562
sqft_living15    0.270071
sqft_above       0.258919
bathrooms        0.205687
sqft_lot15       0.084961
bedrooms         0.080456
floors           0.078557
yr_built         0.074420
sqft_basement    0.066095
```

```
sqft_lot         0.060936
view             0.054255
waterfront       0.012395
yr_renovated     0.012091
condition        0.011701
dtype: float64
```

[8]:
```
X = X_all.loc[:, mi_reg.iloc[:10].index]
```

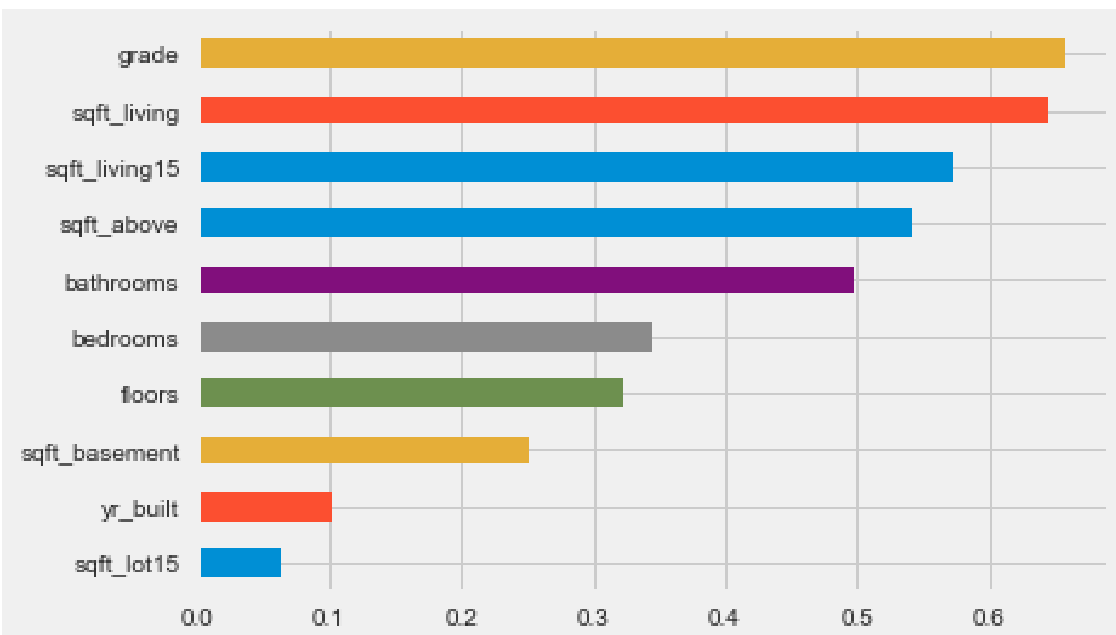
1.2.4 Bivariate Scatter Plots

[9]:
```
sns.pairplot(X.assign(price=y), y_vars=['price'], x_vars=X.columns);
```



1.2.5 Explore Correlations

[10]:
```
correl = (X
          .apply(lambda x: spearmanr(x, y))
          .apply(pd.Series, index=['r', 'pval']))

correl.r.sort_values().plot.barh();
```



1.3 KNN Regression

1.3.1 In-sample performance with default settings

KNN uses distance to make predictions; it requires standardization of variables to avoid undue influence based on scale

[11]:
```
X_scaled = scale(X)
```

[12]:
```
model = KNeighborsRegressor()
model.fit(X=X_scaled, y=y)
```

[12]:
```
KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='minkowski',
          metric_params=None, n_jobs=None, n_neighbors=5, p=2,
          weights='uniform')
```

[13]:
```
y_pred = model.predict(X_scaled)
```

1.3.2 Regression Error Metrics

[14]:
```
from sklearn.metrics import (mean_squared_error,
                             mean_absolute_error,
                             mean_squared_log_error,
                             median_absolute_error,
                             explained_variance_score,
                             r2_score)
```

Computing the prediction error The error is the deviation from the true value, whereas a residual is the deviation from an estimated value, e.g., an estimate of the population mean.

[15]:
```
error = (y - y_pred).rename('Prediction Errors')
```

[16]:
```
scores = dict(
    rmse=np.sqrt(mean_squared_error(y_true=y, y_pred=y_pred)),
    rmsle=np.sqrt(mean_squared_log_error(y_true=y, y_pred=y_pred)),
    mean_ae=mean_absolute_error(y_true=y, y_pred=y_pred),
    median_ae=median_absolute_error(y_true=y, y_pred=y_pred),
    r2score=explained_variance_score(y_true=y, y_pred=y_pred)
)
```

[17]:
```
fig, axes = plt.subplots(ncols=3, figsize=(15, 5))
sns.scatterplot(x=y, y=y_pred, ax=axes[0])
axes[0].set_xlabel('Log Price')
axes[0].set_ylabel('Predictions')
axes[0].set_ylim(11, 16)
sns.distplot(error, ax=axes[1])
pd.Series(scores).plot.barh(ax=axes[2], title='Error Metrics')
fig.suptitle('In-Sample Regression Errors', fontsize=24)
```

```
fig.tight_layout()
plt.subplots_adjust(top=.8);
```

1.3.3 Cross-Validation

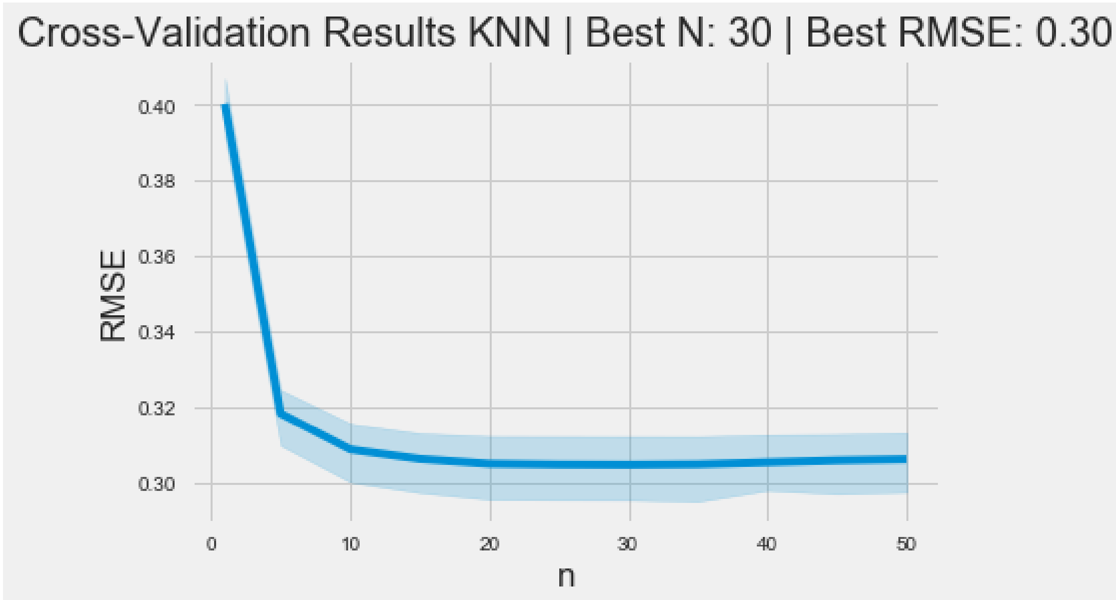
Manual hyperparameter tuning; using [Pipeline](#) ensures proper scaling for each fold using train metrics to standardize test data.

[18]:
```
def rmse(y_true, pred):
    return np.sqrt(mean_squared_error(y_true=y_true, y_pred=pred))

rmse_score = make_scorer(rmse)
```

[22]:
```
cv_rmse = {}
n_neighbors = [1] + list(range(5, 51, 5))
for n in n_neighbors:
    pipe = Pipeline([('scaler', StandardScaler()),
                     ('knn', KNeighborsRegressor(n_neighbors=n))])
    cv_rmse[n] = cross_val_score(pipe,
                                 X=X,
                                 y=y,
                                 scoring=rmse_score,
                                 cv=5)
```

[23]:
```
cv_rmse = pd.DataFrame.from_dict(cv_rmse, orient='index')
best_n, best_rmse = cv_rmse.mean(1).idxmin(), cv_rmse.mean(1).min()
cv_rmse = cv_rmse.stack().reset_index()
cv_rmse.columns =['n', 'fold', 'RMSE']
```

[24]:
```
ax = sns.lineplot(x='n', y='RMSE', data=cv_rmse)
ax.set_title(f'Cross-Validation Results KNN | Best N: {best_n:d} | Best RMSE:␣
 ↪{best_rmse:.2f}');
```



Actuals vs Predicted

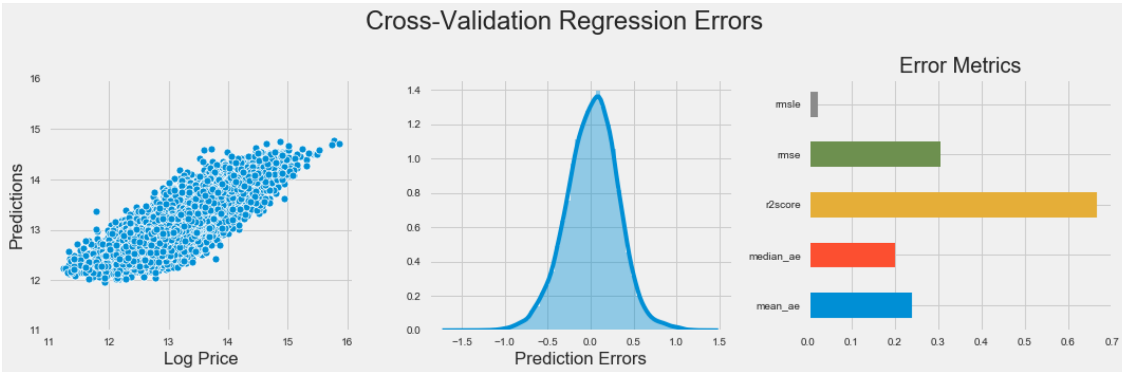
[25]:
```
pipe = Pipeline([('scaler', StandardScaler()),
                 ('knn', KNeighborsRegressor(n_neighbors=best_n))])
y_pred = cross_val_predict(pipe, X, y, cv=5)

ax = sns.scatterplot(x=y, y=y_pred)
y_range = list(range(int(y.min() + 1), int(y.max() + 1)))
pd.Series(y_range, index=y_range).plot(ax=ax, lw=2, c='darkred');
```

Cross-Validation Errors

[26]:
```
error = (y - y_pred).rename('Prediction Errors')
```

[27]:
```
scores = dict(
    rmse=np.sqrt(mean_squared_error(y_true=y, y_pred=y_pred)),
    rmsle=np.sqrt(mean_squared_log_error(y_true=y, y_pred=y_pred)),
    mean_ae=mean_absolute_error(y_true=y, y_pred=y_pred),
    median_ae=median_absolute_error(y_true=y, y_pred=y_pred),
    r2score=explained_variance_score(y_true=y, y_pred=y_pred)
)
```

[28]:
```
fig, axes = plt.subplots(ncols=3, figsize=(15, 5))
sns.scatterplot(x=y, y=y_pred, ax=axes[0])
axes[0].set_xlabel('Log Price')
axes[0].set_ylabel('Predictions')
axes[0].set_ylim(11, 16)
sns.distplot(error, ax=axes[1])
pd.Series(scores).plot.barh(ax=axes[2], title='Error Metrics')
fig.suptitle('Cross-Validation Regression Errors', fontsize=24)
fig.tight_layout()
plt.subplots_adjust(top=.8);
```



1.3.4 GridSearchCV with Pipeline

See sklearn docs.

[30]:
```
pipe = Pipeline([('scaler', StandardScaler()),
                 ('knn', KNeighborsRegressor())])

n_folds = 5
n_neighbors = tuple(range(5, 101, 5))

param_grid = {'knn__n_neighbors': n_neighbors}

estimator = GridSearchCV(estimator=pipe,
                         param_grid=param_grid,
                         cv=n_folds,
                         scoring=rmse_score,
#                          n_jobs=-1
                        )
estimator.fit(X=X, y=y)
```

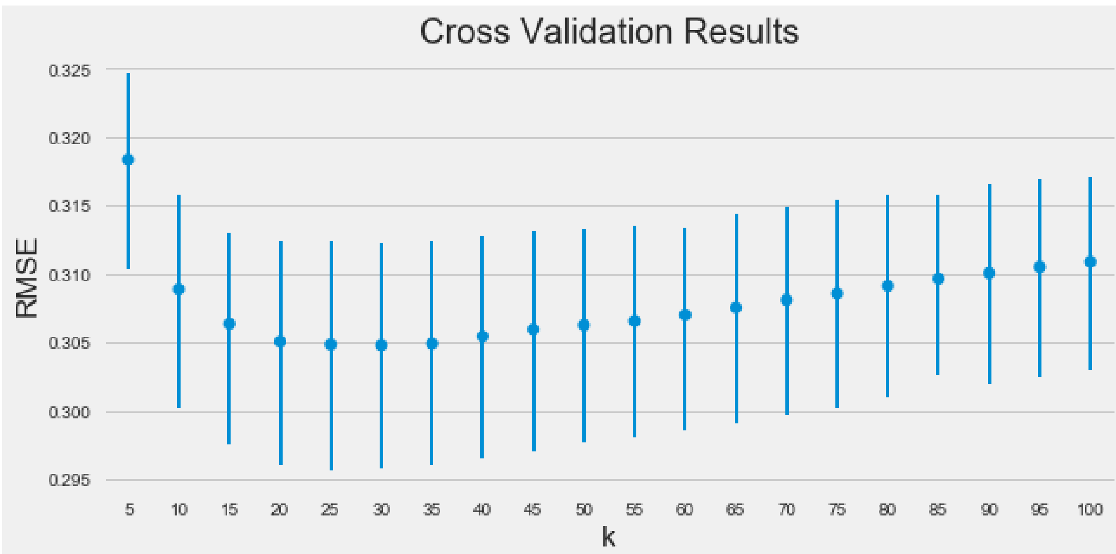
[30]:
```
GridSearchCV(cv=5, error_score='raise-deprecating',
       estimator=Pipeline(memory=None,
     steps=[('scaler', StandardScaler(copy=True, with_mean=True,
with_std=True)), ('knn', KNeighborsRegressor(algorithm='auto', leaf_size=30,
metric='minkowski',
          metric_params=None, n_jobs=None, n_neighbors=5, p=2,
          weights='uniform'))]),
       fit_params=None, iid='warn', n_jobs=None,
       param_grid={'knn__n_neighbors': (5, 10, 15, 20, 25, 30, 35, 40, 45, 50,
55, 60, 65, 70, 75, 80, 85, 90, 95, 100)},
       pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
       scoring=make_scorer(rmse), verbose=0)
```

[31]:
```
cv_results = estimator.cv_results_
```

```
[32]: test_scores = pd.DataFrame({fold: cv_results[f'split{fold}_test_score'] for␣
      ↪fold in range(n_folds)},
                                 index=n_neighbors).stack().reset_index()
      test_scores.columns = ['k', 'fold', 'RMSE']
```

```
[33]: mean_rmse = test_scores.groupby('k').RMSE.mean()
      best_k, best_score = mean_rmse.idxmin(), mean_rmse.min()
```

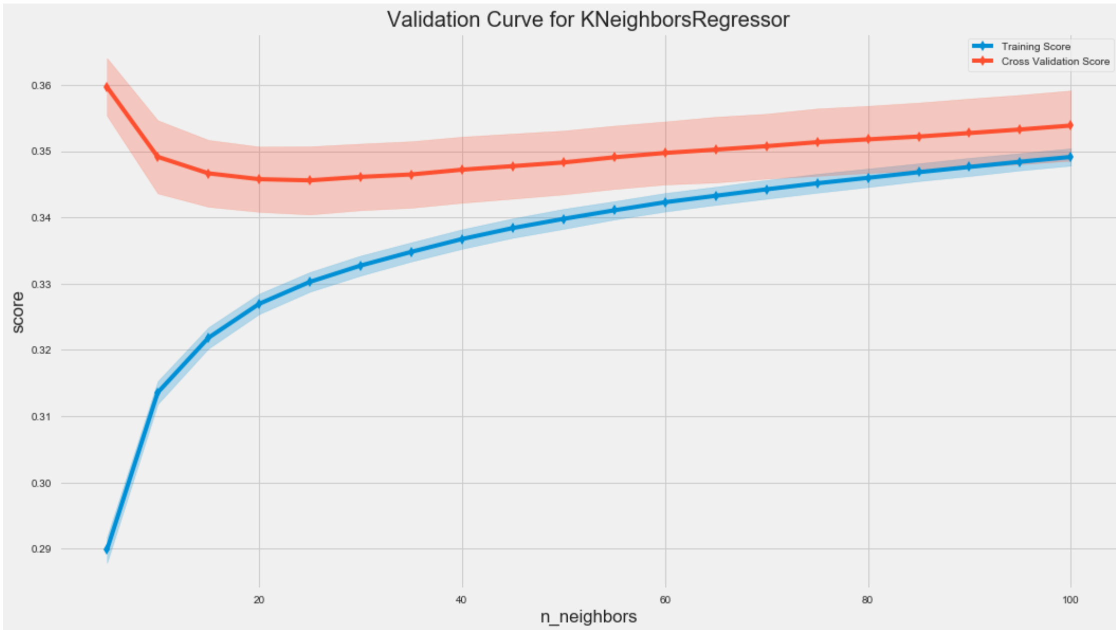
```
[34]: sns.pointplot(x='k', y='RMSE', data=test_scores, scale=.3, join=False,␣
      ↪errwidth=2)
      plt.title('Cross Validation Results')
      plt.tight_layout()
      plt.gcf().set_size_inches(10, 5);
```



1.3.5 Train & Validation Curves mit yellowbricks

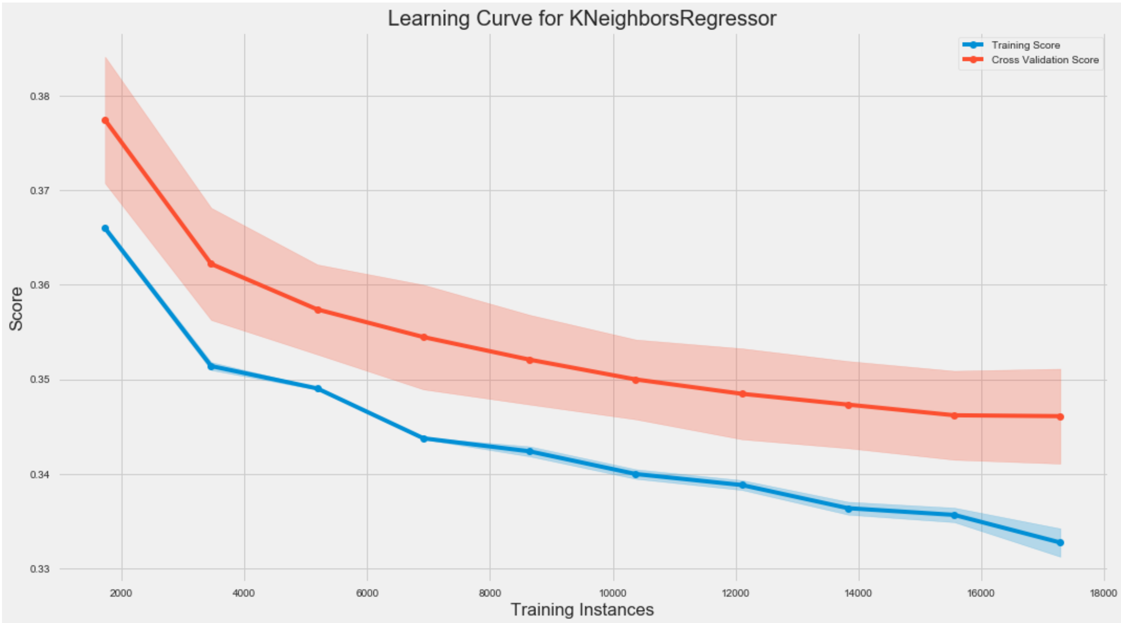
See background on learning curves and yellowbrick docs.

```
[35]: fig, ax = plt.subplots(figsize=(16, 9))
      val_curve = ValidationCurve(KNeighborsRegressor(),
                            param_name='n_neighbors',
                            param_range=n_neighbors,
                            cv=5,
                            scoring=rmse_score,
      #                       n_jobs=-1,
                            ax=ax)
      val_curve.fit(X, y)
      val_curve.poof()
      fig.tight_layout();
```



[36]:

```
fig, ax = plt.subplots(figsize=(16, 9))
l_curve = LearningCurve(KNeighborsRegressor(n_neighbors=best_k),
                        train_sizes=np.arange(.1, 1.01, .1),
                        scoring=rmse_score,
                        cv=5,
#                         n_jobs=-1,
                        ax=ax)
l_curve.fit(X, y)
l_curve.poof()
fig.tight_layout();
```



1.4 Binary Classification

[37]:
```
y_binary = (y>y.median()).astype(int)
```

[38]:
```
n_neighbors = tuple(range(5, 151, 10))
n_folds = 5
scoring = 'roc_auc'
```

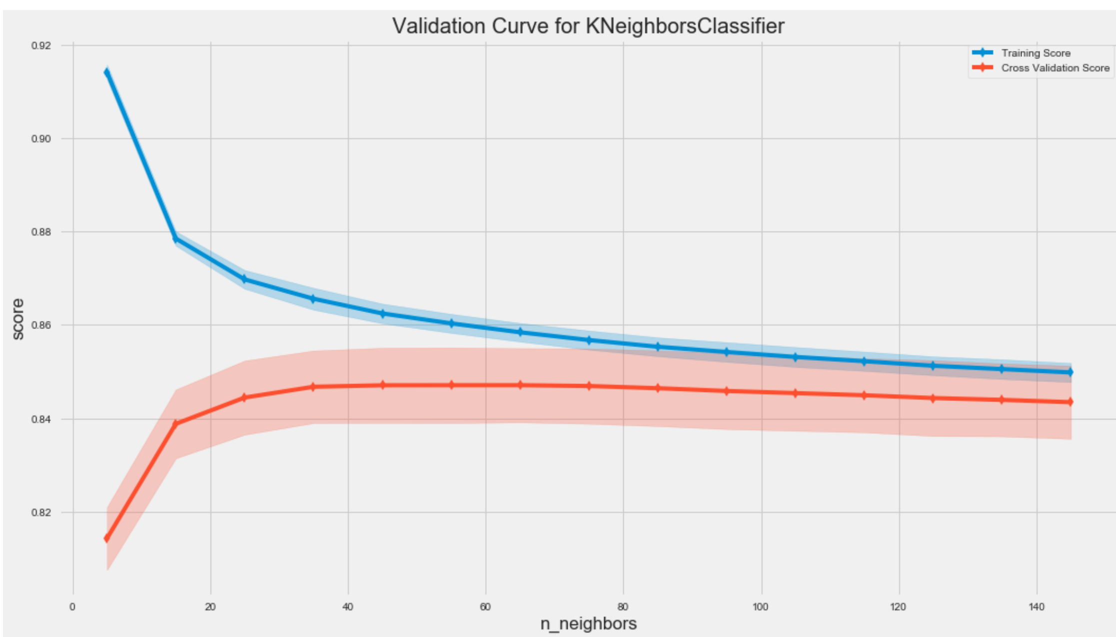
[39]:
```
pipe = Pipeline([('scaler', StandardScaler()),
                 ('knn', KNeighborsClassifier())])

param_grid = {'knn__n_neighbors': n_neighbors}

estimator = GridSearchCV(estimator=pipe,
                         param_grid=param_grid,
                         cv=n_folds,
                         scoring=scoring,
#                          n_jobs=-1
                        )
estimator.fit(X=X, y=y_binary)
```

[39]:
```
GridSearchCV(cv=5, error_score='raise-deprecating',
       estimator=Pipeline(memory=None,
     steps=[('scaler', StandardScaler(copy=True, with_mean=True,
with_std=True)), ('knn', KNeighborsClassifier(algorithm='auto', leaf_size=30,
metric='minkowski',
```

```
            metric_params=None, n_jobs=None, n_neighbors=5, p=2,
            weights='uniform'))]),
        fit_params=None, iid='warn', n_jobs=None,
        param_grid={'knn__n_neighbors': (5, 15, 25, 35, 45, 55, 65, 75, 85, 95,
105, 115, 125, 135, 145)},
        pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
        scoring='roc_auc', verbose=0)
```

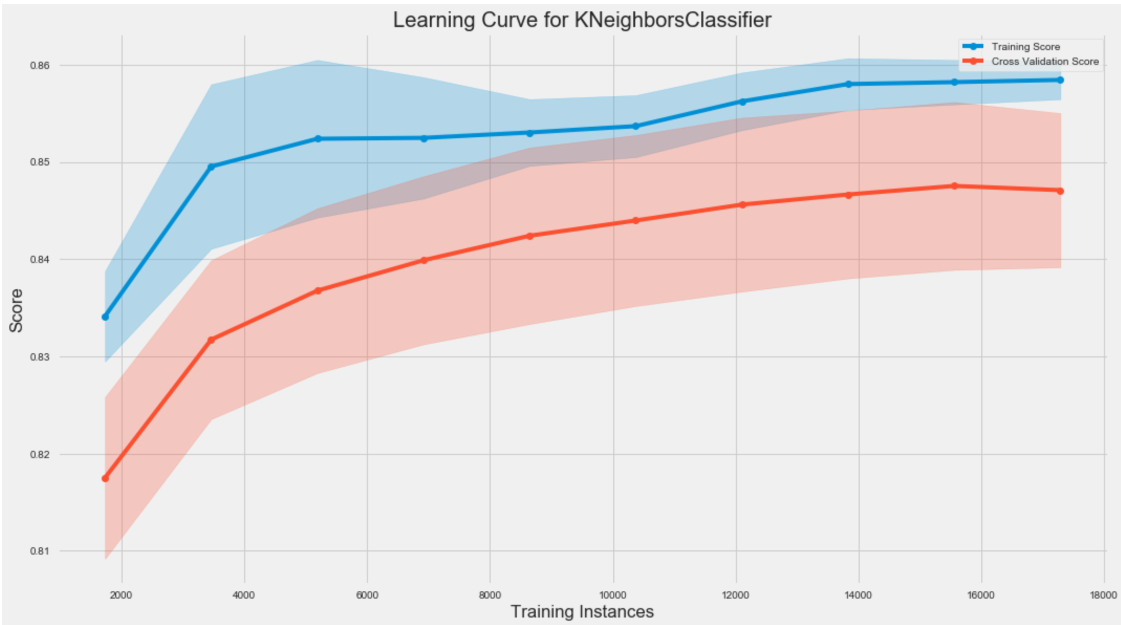
[40]:
```
best_k = estimator.best_params_['knn__n_neighbors']
```

[41]:
```
fig, ax = plt.subplots(figsize=(16, 9))
val_curve = ValidationCurve(KNeighborsClassifier(),
                      param_name='n_neighbors',
                      param_range=n_neighbors,
                      cv=n_folds,
                      scoring=scoring,
#                       n_jobs=-1,
                      ax=ax)
val_curve.fit(X, y_binary)
val_curve.poof()
fig.tight_layout();
```



[42]:
```
fig, ax = plt.subplots(figsize=(16, 9))
l_curve = LearningCurve(KNeighborsClassifier(n_neighbors=best_k),
                        train_sizes=np.arange(.1, 1.01, .1),
                        scoring=scoring,
```

```
                            cv=5,
#                             n_jobs=-1,
                            ax=ax)
l_curve.fit(X, y_binary)
l_curve.poof()
fig.tight_layout();
```



1.4.1 Classification Metrics

See sklearn docs for details.

[43]:
```
from sklearn.metrics import (classification_report,
                             accuracy_score,
                             zero_one_loss,
                             auc,
                             roc_auc_score,
                             roc_curve,
                             brier_score_loss,
                             cohen_kappa_score,
                             confusion_matrix,
                             fbeta_score,
                             hamming_loss,
                             hinge_loss,
                             jaccard_similarity_score,
                             log_loss,
                             matthews_corrcoef,
                             f1_score,
```

```
                              precision_recall_fscore_support,
                              average_precision_score,
                              precision_recall_curve,
                              precision_score,
                              recall_score)
```

Name	API
Area Under the Receiver Operating Characteristic Curve (ROC AUC)	roc_auc_score(y_true, y_score[, …])
Receiver operating characteristic (ROC)	roc_curve(y_true, y_score[, …])
Average precision (AP)	average_precision_score(y_true, y_score)
Precision-recall pairs	precision_recall_curve(y_true, …)
Precision, recall, F-measure and support	precision_recall_fscore_support(…)
F1 Score	f1_score(y_true, y_pred[, labels, …])
F-beta Score	fbeta_score(y_true, y_pred, beta[, …])
Precision	precision_score(y_true, y_pred[, …]
Recall	recall_score(y_true, y_pred[, …])
Main classification metrics	classification_report(y_true, y_pred)
confusion matrix	confusion_matrix(y_true, y_pred[, …])
Accuracy classification score	accuracy_score(y_true, y_pred)
Zero-one classification loss	zero_one_loss(y_true, y_pred[, …])
Average Hamming loss	hamming_loss(y_true, y_pred[, …])
Brier score	brier_score_loss(y_true, y_prob[, …])
Cohen's kappa	cohen_kappa_score(y1, y2[, labels, …])
Average hinge loss	hinge_loss(y_true, pred_decision[, …])
Jaccard similarity coefficient	jaccard_similarity_score(y_true, y_pred)
Log loss, aka logistic loss or cross-entropy loss	log_loss(y_true, y_pred[, eps, …])
Matthews correlation coefficient (MCC)	matthews_corrcoef(y_true, y_pred[, …])

[44]:
```
y_score = cross_val_predict(KNeighborsClassifier(best_k),
                            X=X,
                            y=y_binary,
                            cv=5,
#                             n_jobs=-1,
                            method='predict_proba')[:, 1]
```

Using Predicted Probabilities

[46]:
```
pred_scores = dict(y_true=y_binary,y_score=y_score)
```

ROC AUC

[47]:
```
roc_auc_score(**pred_scores)
```

[47]: 0.8460203973490154

[48]:
```python
cols = ['False Positive Rate', 'True Positive Rate', 'threshold']
roc = pd.DataFrame(dict(zip(cols, roc_curve(**pred_scores))))
```

Precision-Recall

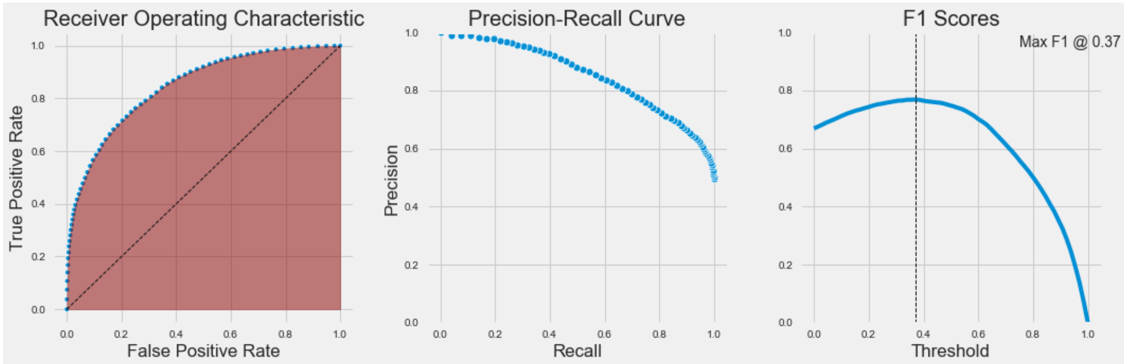
[49]:
```python
precision, recall, ts = precision_recall_curve(y_true=y_binary,␣
↪probas_pred=y_score)
pr_curve = pd.DataFrame({'Precision': precision, 'Recall': recall})
```

F1 Score - Optimize Threshold

[52]:
```python
f1 = pd.Series({t: f1_score(y_true=y_binary, y_pred=y_score>t) for t in ts})
best_threshold = f1.idxmax()
```

Plot

[53]:
```python
fig, axes = plt.subplots(ncols=3, figsize=(15, 5))

ax = sns.scatterplot(x='False Positive Rate', y='True Positive Rate', data=roc,␣
↪size=5, legend=False, ax=axes[0])
axes[0].plot(np.linspace(0,1,100), np.linspace(0,1,100), color='k', ls='--',␣
↪lw=1)
axes[0].fill_between(y1=roc['True Positive Rate'], x=roc['False Positive␣
↪Rate'], alpha=.5,color='darkred')
axes[0].set_title('Receiver Operating Characteristic')


sns.scatterplot(x='Recall', y='Precision', data=pr_curve, ax=axes[1])
axes[1].set_ylim(0,1)
axes[1].set_title('Precision-Recall Curve')


f1.plot(ax=axes[2], title='F1 Scores', ylim=(0,1))
axes[2].set_xlabel('Threshold')
axes[2].axvline(best_threshold, lw=1, ls='--', color='k')
axes[2].text(text=f'Max F1 @ {best_threshold:.2f}', x=.75, y=.95, s=5)
fig.tight_layout();
```



Average Precision

```
[54]: average_precision_score(y_true=y_binary, y_score=y_score)
```

```
[54]: 0.8484062482212291
```

Brier Score

```
[55]: brier_score_loss(y_true=y_binary, y_prob=y_score)
```

```
[55]: 0.16022915202525762
```

Use Predictions after thresholding

```
[56]: y_pred = y_score > best_threshold
```

```
[57]: scores = dict(y_true=y_binary, y_pred=y_pred)
```

F-beta Score

```
[58]: fbeta_score(**scores, beta=1)
```

```
[58]: 0.768433805405857
```

```
[59]: print(classification_report(**scores))
```

```
              precision    recall  f1-score   support

           0       0.82      0.63      0.71     10864
           1       0.70      0.86      0.77     10749

   micro avg       0.74      0.74      0.74     21613
   macro avg       0.76      0.74      0.74     21613
weighted avg       0.76      0.74      0.74     21613
```

Confusion Matrix

[60]:
```
confusion_matrix(**scores)
```

[60]:
```
array([[6873, 3991],
       [1552, 9197]])
```

Accuracy

[61]:
```
accuracy_score(**scores)
```

[61]:
```
0.7435339841761902
```

Zero-One Loss

[62]:
```
zero_one_loss(**scores)
```

[62]:
```
0.2564660158238098
```

Hamming Loss Fraction of labels that are incorrectly predicted

[63]:
```
hamming_loss(**scores)
```

[63]:
```
0.25646601582380973
```

Cohen's Kappa Score that expresses the level of agreement between two annotators on a classification problem.

[64]:
```
cohen_kappa_score(y1=y_binary, y2=y_pred)
```

[64]:
```
0.4876687258259045
```

Hinge Loss

[65]:
```
hinge_loss(y_true=y_binary, pred_decision=y_pred)
```

[65]:
```
0.7591264516726044
```

Jaccard Similarity

[66]:
```
jaccard_similarity_score(**scores)
```

[66]:
```
0.7435339841761902
```

Log Loss / Cross Entropy Loss

[67]:
```
log_loss(**scores)
```

[67]:
```
8.858170025000408
```

Matthews Correlation Coefficient

[68]:
```
matthews_corrcoef(**scores)
```

[68]:
```
0.5005536590342685
```

1.5 Multi-Class

[69]:
```
y_multi = pd.qcut(y, q=3, labels=[0,1,2])
```

[70]:
```
n_neighbors = tuple(range(5, 151, 10))
n_folds = 5
scoring = 'accuracy'
```

[71]:
```
pipe = Pipeline([('scaler', StandardScaler()),
                 ('knn', KNeighborsClassifier())])

param_grid = {'knn__n_neighbors': n_neighbors}

estimator = GridSearchCV(estimator=pipe,
                         param_grid=param_grid,
                         cv=n_folds,
#                          n_jobs=-1
                        )
estimator.fit(X=X, y=y_multi)
```

[71]:
```
GridSearchCV(cv=5, error_score='raise-deprecating',
       estimator=Pipeline(memory=None,
     steps=[('scaler', StandardScaler(copy=True, with_mean=True,
with_std=True)), ('knn', KNeighborsClassifier(algorithm='auto', leaf_size=30,
metric='minkowski',
           metric_params=None, n_jobs=None, n_neighbors=5, p=2,
           weights='uniform'))]),
       fit_params=None, iid='warn', n_jobs=None,
       param_grid={'knn__n_neighbors': (5, 15, 25, 35, 45, 55, 65, 75, 85, 95,
105, 115, 125, 135, 145)},
       pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
       scoring=None, verbose=0)
```

[72]:
```
y_pred = cross_val_predict(estimator.best_estimator_,
                           X=X,
                           y=y_multi,
                           cv=5,
#                            n_jobs=-1,
                           method='predict')
```

[73]:
```
print(classification_report(y_true=y_multi, y_pred=y_pred))
```

```
              precision    recall  f1-score   support

           0       0.67      0.71      0.69      7226
           1       0.52      0.52      0.52      7223
           2       0.77      0.74      0.75      7164

   micro avg       0.65      0.65      0.65     21613
   macro avg       0.65      0.65      0.65     21613
weighted avg       0.65      0.65      0.65     21613
```

[ ]: