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
warnings.filterwarnings('ignore')
```

[2]:
```
%matplotlib inline

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,
                                     GridSearchCV)
from sklearn.feature_selection import mutual_info_regression
from sklearn.preprocessing import StandardScaler, scale
from sklearn.pipeline import Pipeline
from sklearn.metrics import make_scorer
from yellowbrick.model_selection import ValidationCurve, LearningCurve
```

[3]:
```
sns.set_style('whitegrid')
```

1.1 Get the Data

1.1.1 Kings County Housing Data

Data from Kaggle

Download via API:

`kaggle datasets download -d harlfoxem/housesalesprediction`

[4]:
```
DATA_PATH = Path('..', 'data')
```

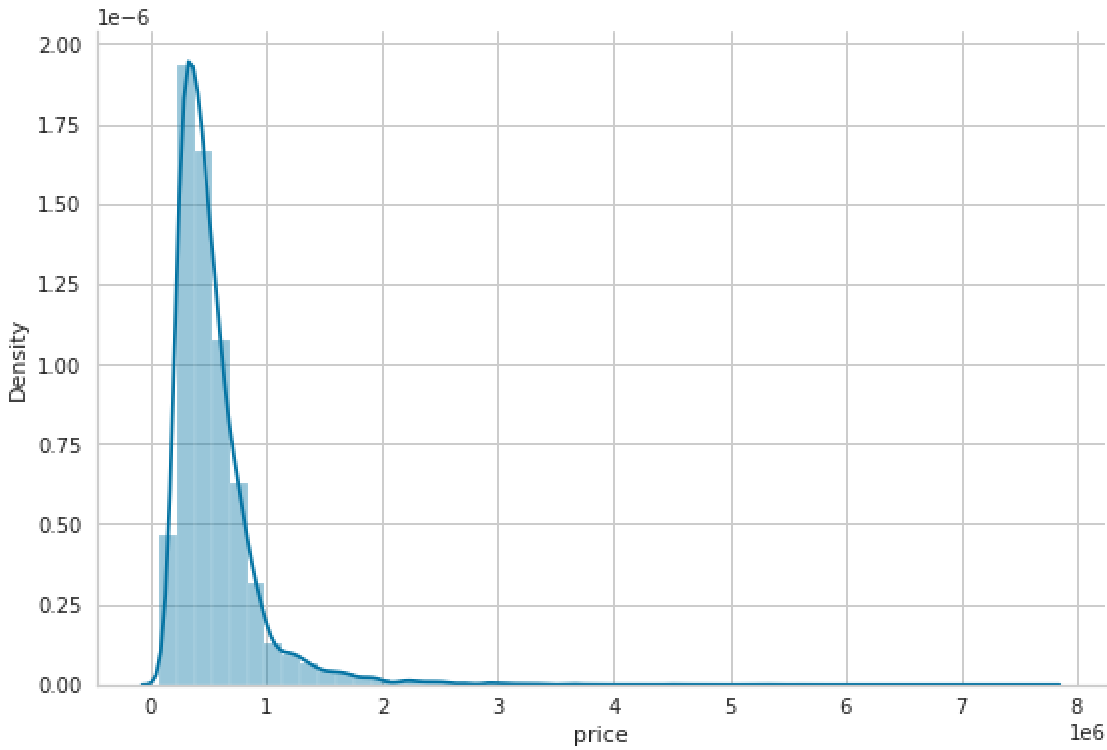
[5]:
```
house_sales = pd.read_csv('kc_house_data.csv')
house_sales = house_sales.drop(
    ['id', 'zipcode', 'lat', 'long', 'date'], axis=1)
house_sales.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 21613 entries, 0 to 21612
Data columns (total 16 columns):
 #   Column         Non-Null Count  Dtype
---  ------         --------------  -----
 0   price          21613 non-null  float64
 1   bedrooms       21613 non-null  int64
 2   bathrooms      21613 non-null  float64
 3   sqft_living    21613 non-null  int64
 4   sqft_lot       21613 non-null  int64
 5   floors         21613 non-null  float64
 6   waterfront     21613 non-null  int64
 7   view           21613 non-null  int64
 8   condition      21613 non-null  int64
 9   grade          21613 non-null  int64
 10  sqft_above     21613 non-null  int64
 11  sqft_basement  21613 non-null  int64
 12  yr_built       21613 non-null  int64
 13  yr_renovated   21613 non-null  int64
 14  sqft_living15  21613 non-null  int64
 15  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

[6]:
```
sns.distplot(house_sales.price)
sns.despine()
plt.tight_layout();
```



1.2.2 Use log-transform

Useful for dealing with skewed data.

[7]:
```
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.

[8]:
```
mi_reg = pd.Series(mutual_info_regression(X_all, y),
                   index=X_all.columns).sort_values(ascending=False)
mi_reg
```

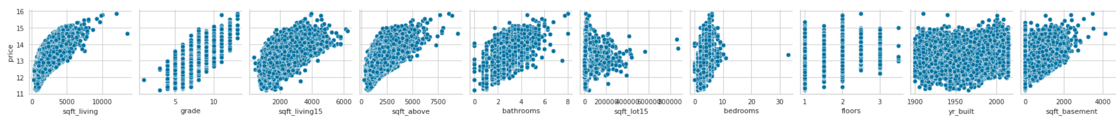
[8]:
```
sqft_living      0.347760
grade            0.342861
sqft_living15    0.269146
sqft_above       0.258574
bathrooms        0.202894
sqft_lot15       0.085729
bedrooms         0.079577
floors           0.078963
```

```
yr_built         0.076893
sqft_basement    0.069330
sqft_lot         0.062372
view             0.058605
waterfront       0.010809
yr_renovated     0.009336
condition        0.004629
dtype: float64
```

[9]:
```python
X = X_all.loc[:, mi_reg.iloc[:10].index]
```

1.2.4 Bivariate Scatter Plots

[10]:
```python
g = sns.pairplot(X.assign(price=y), y_vars=['price'], x_vars=X.columns)
sns.despine();
```

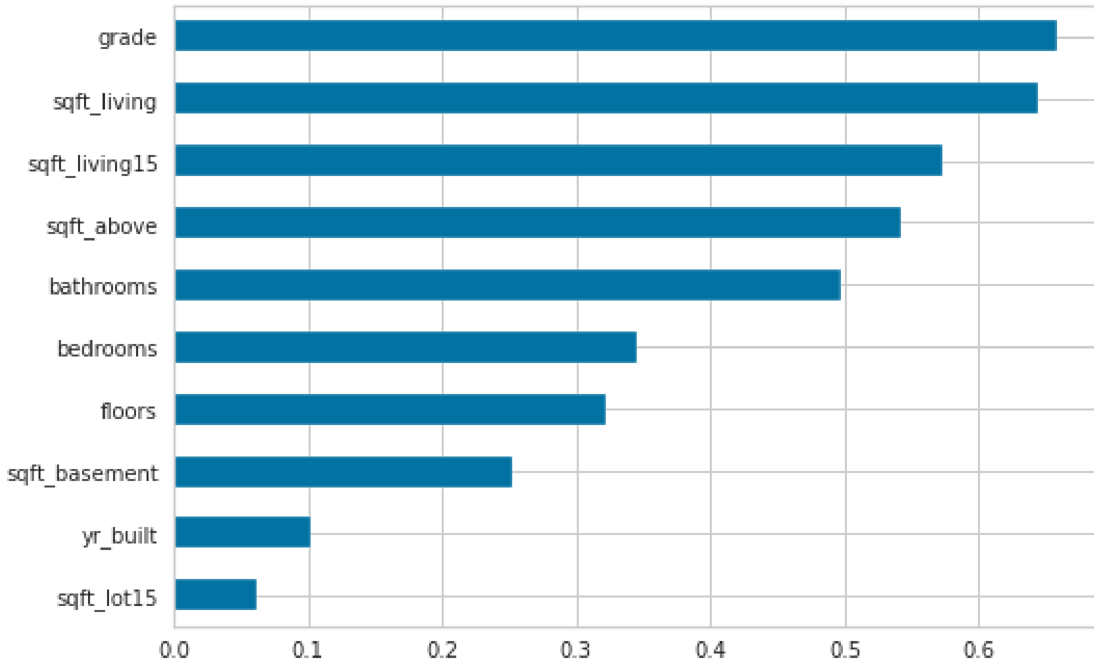


1.2.5 Explore Correlations

[11]:
```python
X.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 21613 entries, 0 to 21612
Data columns (total 10 columns):
 #   Column         Non-Null Count  Dtype
---  ------         --------------  -----
 0   sqft_living    21613 non-null  int64
 1   grade          21613 non-null  int64
 2   sqft_living15  21613 non-null  int64
 3   sqft_above     21613 non-null  int64
 4   bathrooms      21613 non-null  float64
 5   sqft_lot15     21613 non-null  int64
 6   bedrooms       21613 non-null  int64
 7   floors         21613 non-null  float64
 8   yr_built       21613 non-null  int64
 9   sqft_basement  21613 non-null  int64
dtypes: float64(2), int64(8)
memory usage: 1.6 MB
```

[12]:
```python
correl = X.apply(lambda x: spearmanr(x, y)[0])
correl.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

[13]:
```
X_scaled = scale(X)
```

[14]:
```
model = KNeighborsRegressor()
model.fit(X=X_scaled, y=y)
```

[14]: KNeighborsRegressor()

[15]:
```
y_pred = model.predict(X_scaled)
```

1.3.2 Regression Error Metrics

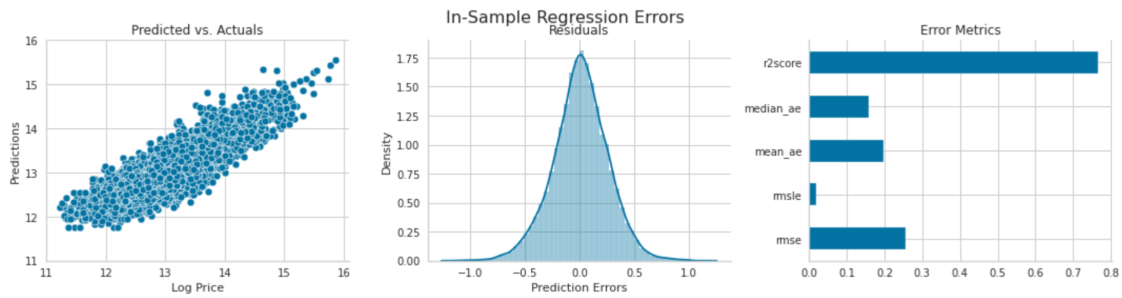
[16]:
```
from sklearn.metrics import (mean_squared_error,
                             mean_absolute_error,
                             mean_squared_log_error,
                             median_absolute_error,
                             explained_variance_score,
                             r2_score)
```

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.

[17]:
```
error = (y - y_pred).rename('Prediction Errors')
```

[18]:
```
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)
)
```

[19]:
```
fig, axes = plt.subplots(ncols=3, figsize=(15, 4))
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)
axes[0].set_title('Predicted vs. Actuals')
sns.distplot(error, ax=axes[1])
axes[1].set_title('Residuals')
pd.Series(scores).plot.barh(ax=axes[2], title='Error Metrics')
fig.suptitle('In-Sample Regression Errors', fontsize=16)
sns.despine()
fig.tight_layout()
fig.subplots_adjust(top=.88)
```



1.3.3 Cross-Validation

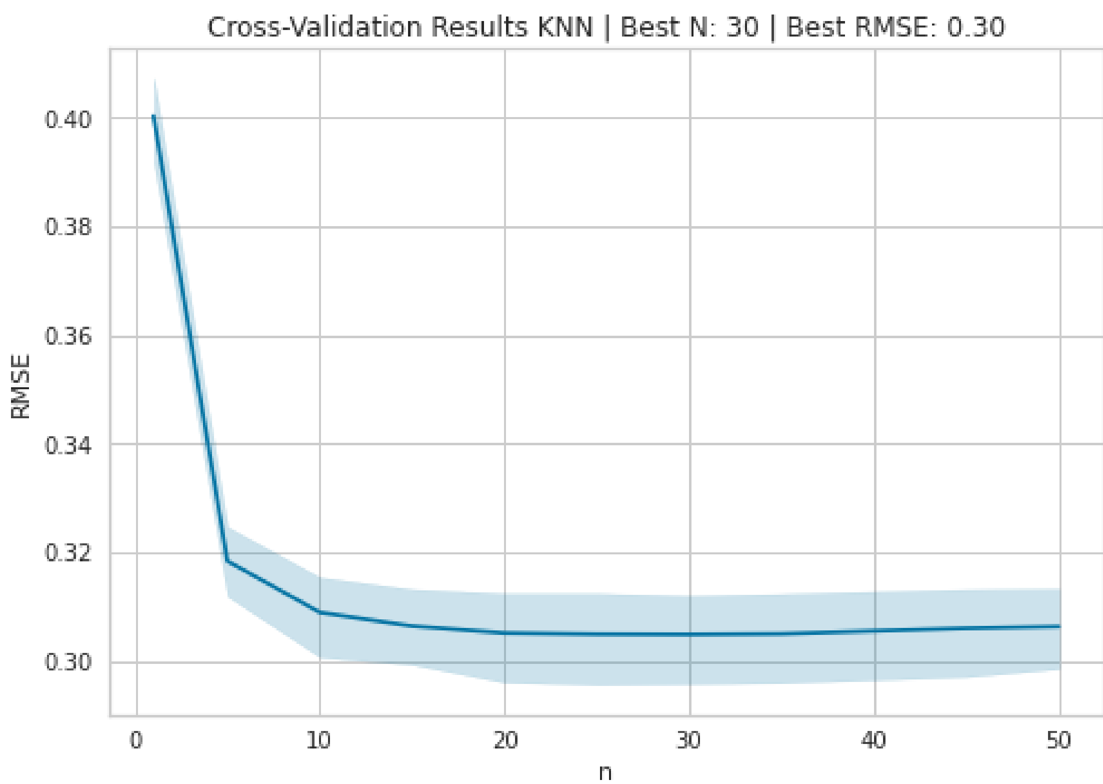
Manual hyperparameter tuning; using Pipeline ensures proper scaling for each fold using train metrics to standardize test data.

[20]:
```
def rmse(y_true, pred):
    return np.sqrt(mean_squared_error(y_true=y_true, y_pred=pred))

rmse_score = make_scorer(rmse)
```

[21]:
```
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)
```

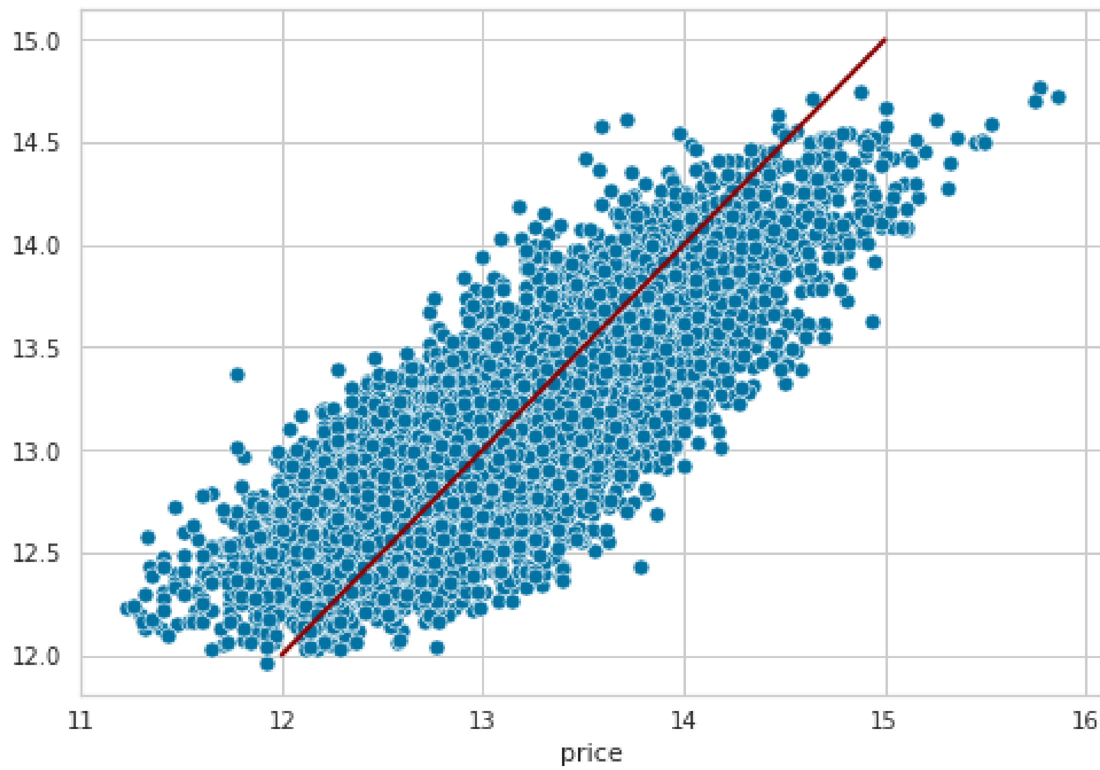
[22]:
```
cv_rmse = pd.DataFrame.from_dict(cv_rmse, orient='index')
best_n, best_rmse = cv_rmse.mean(1).idxmin(), cv_rmse.mean(1).min()
cv_rmse = cv_rmse.stack().reset_index()
cv_rmse.columns =['n', 'fold', 'RMSE']
```

[23]:
```
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

[24]:
```
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');
```



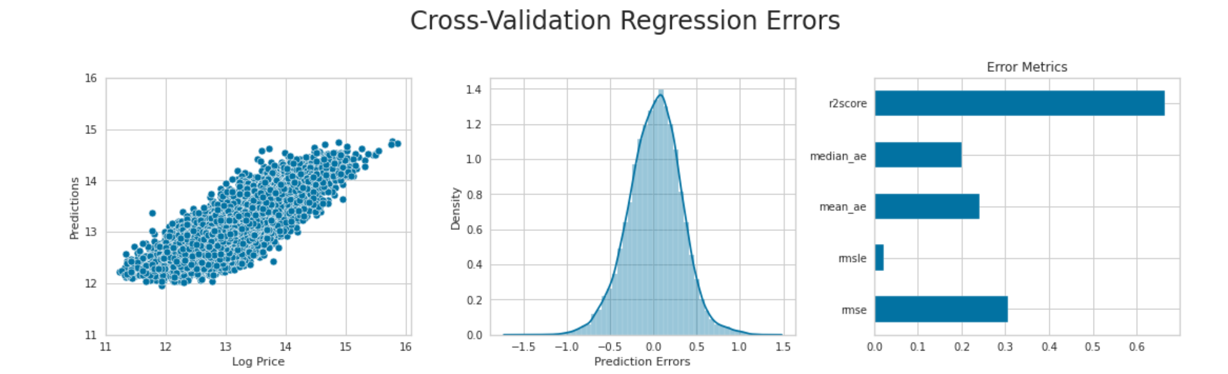
Cross-Validation Errors

[25]:
```
error = (y - y_pred).rename('Prediction Errors')
```

[26]:
```
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)
)
```

[27]:
```
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.

[28]:
```
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)
```

[28]:
```
GridSearchCV(cv=5,
             estimator=Pipeline(steps=[('scaler', StandardScaler()),
                                       ('knn', KNeighborsRegressor())]),
             param_grid={'knn__n_neighbors': (5, 10, 15, 20, 25, 30, 35, 40, 45,
                                              50, 55, 60, 65, 70, 75, 80, 85,
```

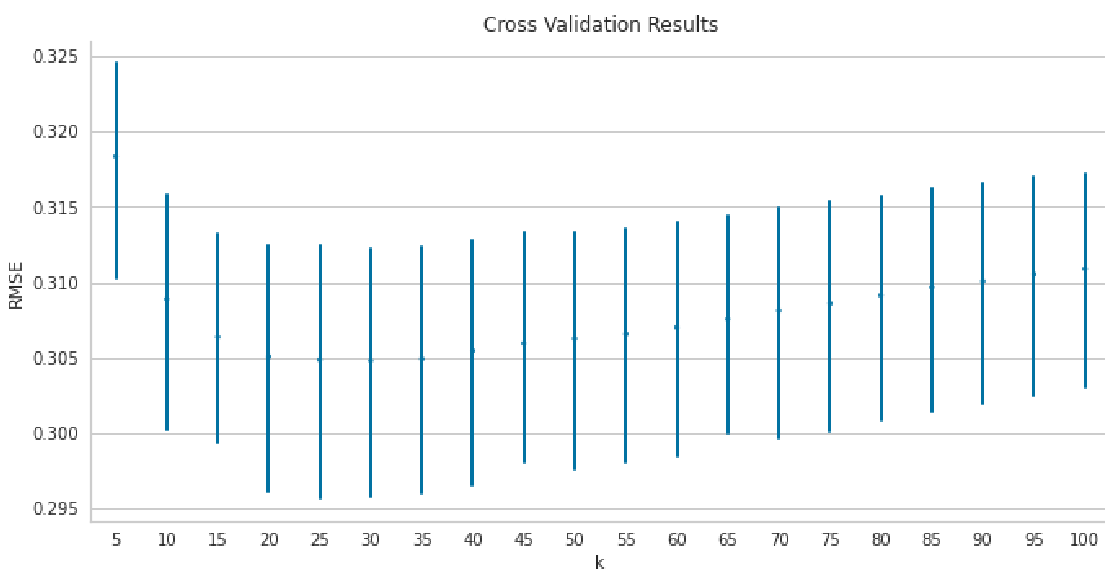
```
                                                                90, 95, 100)},
                         scoring=make_scorer(rmse))
```

[29]:
```
cv_results = estimator.cv_results_
```

[30]:
```
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']
```

[31]:
```
mean_rmse = test_scores.groupby('k').RMSE.mean()
best_k, best_score = mean_rmse.idxmin(), mean_rmse.min()
```

[32]:
```
sns.pointplot(x='k', y='RMSE', data=test_scores, scale=.3, join=False,␣
↪errwidth=2)
plt.title('Cross Validation Results')
sns.despine()
plt.tight_layout()
plt.gcf().set_size_inches(10, 5);
```

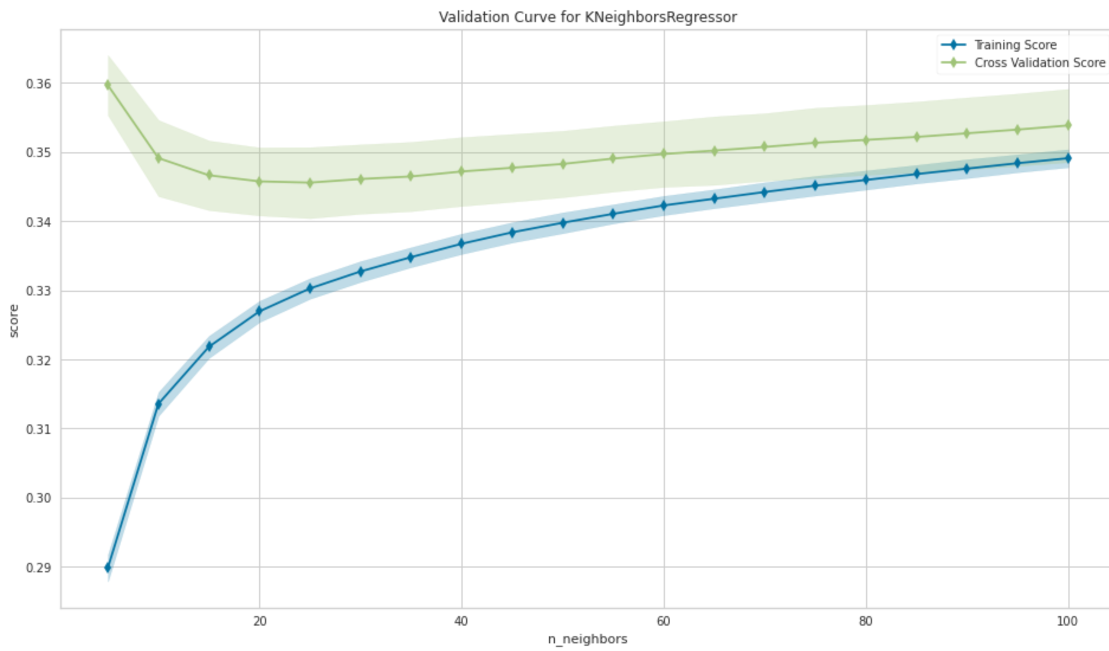


1.3.5 Train & Validation Curves mit yellowbricks

See background on learning curves and yellowbrick docs.

[33]:
```
fig, ax = plt.subplots(figsize=(16, 9))
val_curve = ValidationCurve(KNeighborsRegressor(),
                      param_name='n_neighbors',
                      param_range=n_neighbors,
```

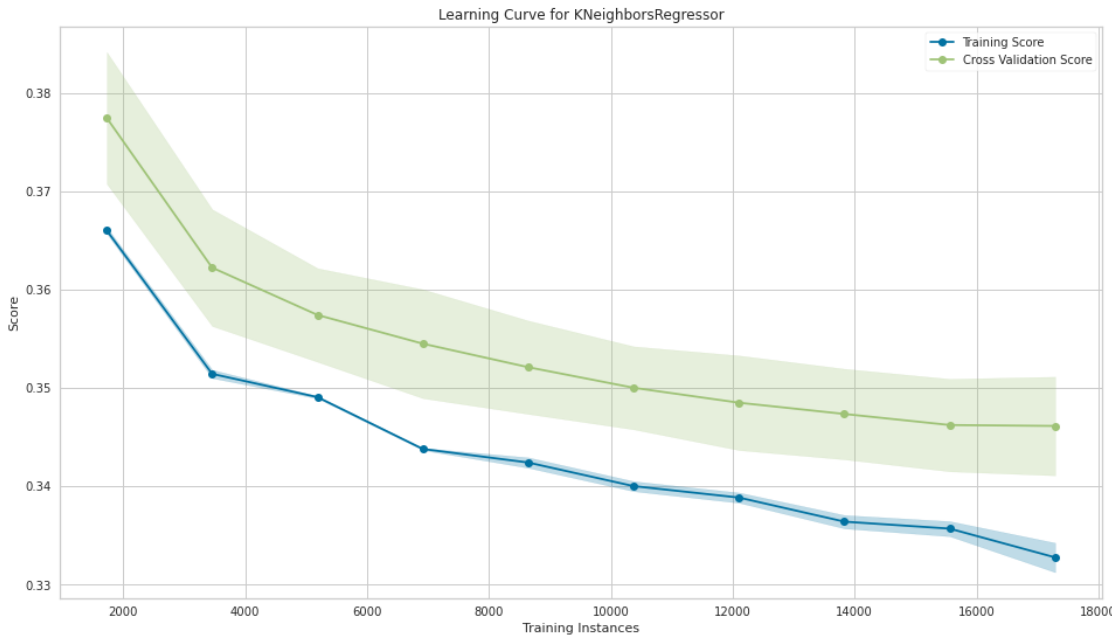
```
                          cv=5,
                          scoring=rmse_score,
#                           n_jobs=-1,
                          ax=ax)
val_curve.fit(X, y)
val_curve.poof()
sns.despine()
fig.tight_layout();
```



<Figure size 576x396 with 0 Axes>

[34]:

```
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()
sns.despine()
fig.tight_layout();
```




```
<Figure size 576x396 with 0 Axes>
```

1.4 Binary Classification

[35]:
```python
y_binary = (y>y.median()).astype(int)
```

[36]:
```python
n_neighbors = tuple(range(5, 151, 10))
n_folds = 5
scoring = 'roc_auc'
```

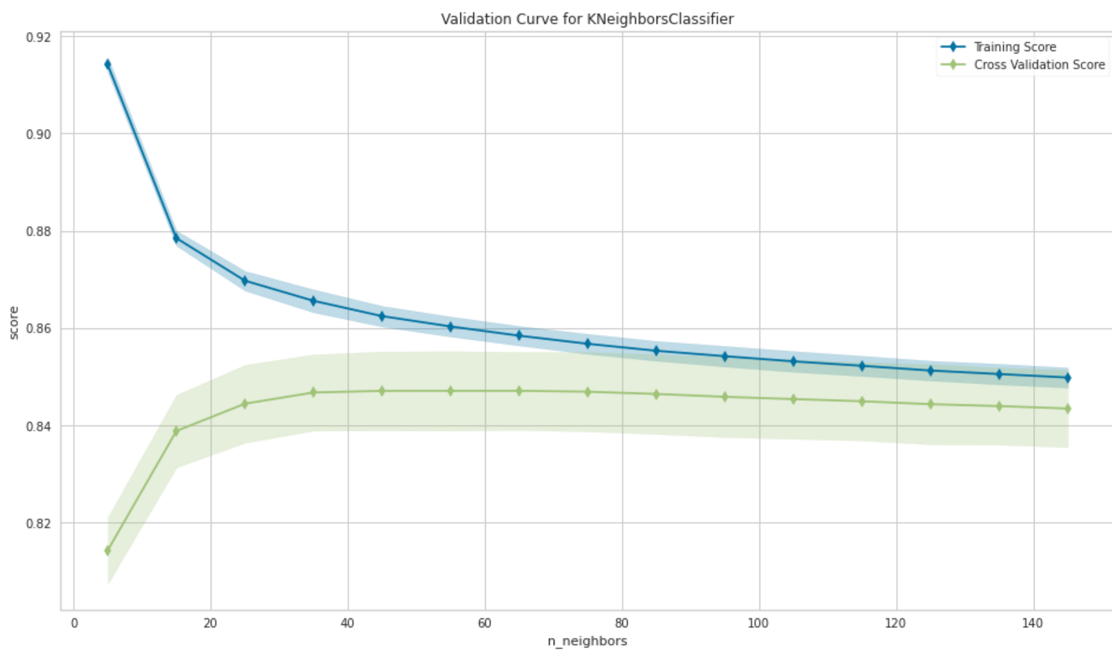
[37]:
```python
pipe = Pipeline([('scaler', StandardScaler()),
                 ('knn', KNeighborsClassifier())])

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)
```

[37]:
```
GridSearchCV(cv=5,
             estimator=Pipeline(steps=[('scaler', StandardScaler()),
                                       ('knn', KNeighborsClassifier())]),
```

```
               param_grid={'knn__n_neighbors': (5, 15, 25, 35, 45, 55, 65, 75, 85,
                                                 95, 105, 115, 125, 135, 145)},
               scoring='roc_auc')
```

[38]:
```
best_k = estimator.best_params_['knn__n_neighbors']
```

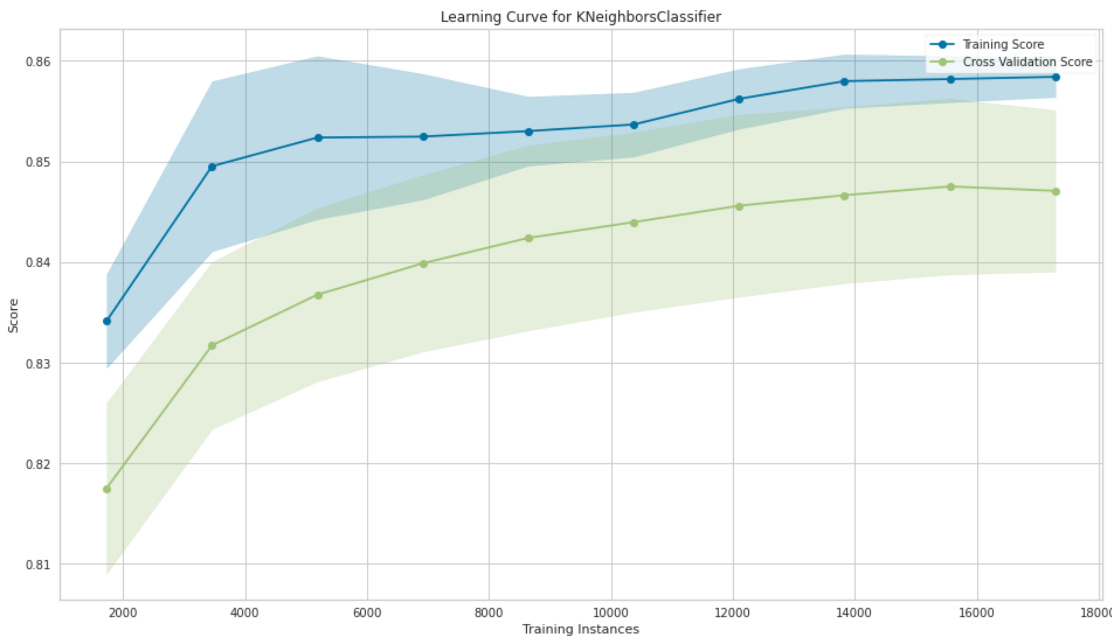
[39]:
```
fig, ax = plt.subplots(figsize=(16, 9))
val_curve = ValidationCurve(KNeighborsClassifier(),
                      param_name='n_neighbors',
                      param_range=n_neighbors,
                      cv=n_folds,
                      scoring=scoring,
#                       n_jobs=-1,
                      ax=ax)
val_curve.fit(X, y_binary)
val_curve.poof()
sns.despine()
fig.tight_layout();
```




```
<Figure size 576x396 with 0 Axes>
```

[40]:
```
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()
sns.despine()
fig.tight_layout();
```



<Figure size 576x396 with 0 Axes>

1.4.1 Classification Metrics

See sklearn docs for details.

[41]:
```
from sklearn.metrics import (classification_report,
                             accuracy_score,
                             zero_one_loss,
                             roc_auc_score,
                             roc_curve,
                             brier_score_loss,
                             cohen_kappa_score,
                             confusion_matrix,
                             fbeta_score,
                             hamming_loss,
                             hinge_loss,
                             jaccard_score,
                             log_loss,
                             matthews_corrcoef,
```

```
                                f1_score,
                                average_precision_score,
                                precision_recall_curve)
```

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[, …])

[42]:
```
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

[43]:
```
pred_scores = dict(y_true=y_binary,y_score=y_score)
```

ROC AUC

[44]:
```
roc_auc_score(**pred_scores)
```

[44]: 0.8460248502754856

[45]:
```
cols = ['False Positive Rate', 'True Positive Rate', 'threshold']
roc = pd.DataFrame(dict(zip(cols, roc_curve(**pred_scores))))
```

Precision-Recall

[46]:
```
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

[47]:
```
f1 = pd.Series({t: f1_score(y_true=y_binary, y_pred=y_score>t) for t in ts})
best_threshold = f1.idxmax()
```

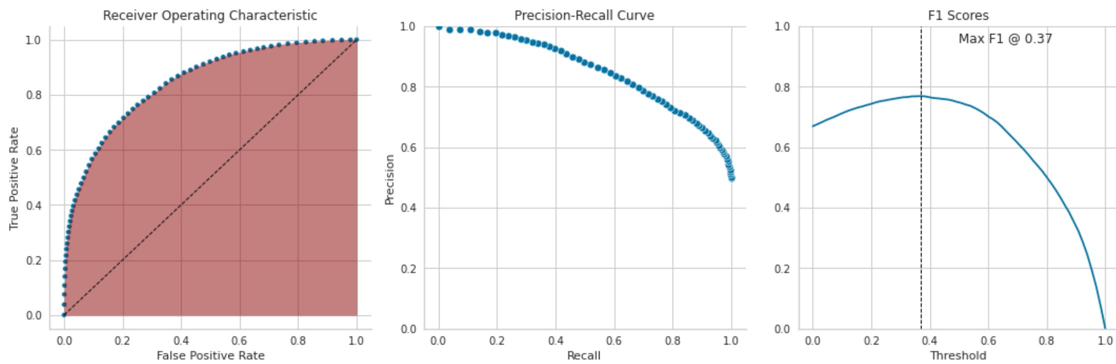
Plot

[48]:
```
roc.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 67 entries, 0 to 66
Data columns (total 3 columns):
 #   Column               Non-Null Count  Dtype
---  ------               --------------  -----
 0   False Positive Rate  67 non-null     float64
 1   True Positive Rate   67 non-null     float64
 2   threshold            67 non-null     float64
dtypes: float64(3)
memory usage: 1.7 KB
```

[49]:
```
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(s=f'Max F1 @ {best_threshold:.2f}', x=.5, y=.95)
sns.despine()
fig.tight_layout();
```



Average Precision

[50]:
```
average_precision_score(y_true=y_binary, y_score=y_score)
```

[50]: 0.8484120767842546

Brier Score

[51]:
```
brier_score_loss(y_true=y_binary, y_prob=y_score)
```

[51]: 0.16022724653171427

Use Predictions after thresholding

[52]:
```
y_pred = y_score > best_threshold
```

[53]:
```
scores = dict(y_true=y_binary, y_pred=y_pred)
```

F-beta Score

[54]:
```
fbeta_score(**scores, beta=1)
```

[54]: 0.7684017044030412

[55]:
```
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
```

```
    accuracy                           0.74     21613
   macro avg       0.76      0.74      0.74     21613
weighted avg       0.76      0.74      0.74     21613
```

Confusion Matrix

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

```
[56]: array([[6872, 3992],
             [1552, 9197]])
```

Accuracy

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

```
[57]: 0.743487715726646
```

Zero-One Loss

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

```
[58]: 0.25651228427335404
```

Hamming Loss Fraction of labels that are incorrectly predicted

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

```
[59]: 0.256512284273354
```

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

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

```
[60]: 0.4875765493181017
```

Hinge Loss

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

```
[61]: 0.7591727201221488
```

Jaccard Similarity

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

```
[62]: 0.6239061122040567
```

Log Loss / Cross Entropy Loss

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

[63]: 8.859768117629491

Matthews Correlation Coefficient

[64]:
```
matthews_corrcoef(**scores)
```

[64]: 0.5004700226167762

1.5 Multi-Class

[65]:
```
y_multi = pd.qcut(y, q=3, labels=[0,1,2])
```

[66]:
```
n_neighbors = tuple(range(5, 151, 10))
n_folds = 5
scoring = 'accuracy'
```

[67]:
```
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)
```

[67]:
```
GridSearchCV(cv=5,
             estimator=Pipeline(steps=[('scaler', StandardScaler()),
                                       ('knn', KNeighborsClassifier())]),
             n_jobs=-1,
             param_grid={'knn__n_neighbors': (5, 15, 25, 35, 45, 55, 65, 75, 85,
                                              95, 105, 115, 125, 135, 145)})
```

[68]:
```
y_pred = cross_val_predict(estimator.best_estimator_,
                           X=X,
                           y=y_multi,
                           cv=5,
                           n_jobs=-1,
                           method='predict')
```

[69]:
```
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
accuracy			0.65	21613
macro avg	0.65	0.65	0.65	21613
weighted avg	0.65	0.65	0.65	21613