XGBoost

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STAT 685: Dr. Suojin Wang's Group

Modeling Seoul Bike Sharing Demand - 003 XGBoosting Study considering Time

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1 Key Takeaways

- Comparing with model assuming independent observation, using anchor date in model training and testing shows a lower performance.
- Information related to time of the year is missing in model training data when an anchor date is set.
- Adding time related attributes has limited improvement.
- Next step:
  - More parameter tuning (Baseline performance is lower than referred literature)
  - Study effect with different anchor day setting and prediction horizon. E.g., predict last few days hourly demand by end of the season; predict next few hours demand in a random day by knowing all information before; etc.

2 Data Process

- Load data and check data format
- Add dummy variables and convert qualitative variable to quantitative
- Randomly select 25% data as testing data

[1]:
```
from numpy import loadtxt
import xgboost as xgb
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score
import os
import time
import pandas as pd
import matplotlib.pyplot as plt
```

[20]:
```
## load data
```

```
fn = os.path.abspath(os.path.join(os.path.dirname(os.getcwd()), './data/
↪SeoulBikeData.csv'))
colNames = ["Date", "RentedBikeCount", "Hour", "Temp", "Humidity", "WindSpeed",␣
↪"Visibility",
            "DewPointTemp", "SolarRadiation","Rainfall", "Snowfall", "Seasons",␣
↪"Holiday", "FunctionalDay"]
dat = pd.read_csv(fn, encoding="ISO-8859-1")
dat.columns = colNames
dat = dat.astype(
    {"Date": str,
    "RentedBikeCount": int,
    "Hour": float,
    "Temp": float,
    "Humidity": float,
    "WindSpeed": float,
    "Visibility": float,
    "DewPointTemp": float,
    "SolarRadiation": float,
    "Rainfall": float,
    "Snowfall": float,
    "Seasons": str,
    "Holiday": str,
    "FunctionalDay": str})

# convert qualitative variable to quantitative
dat = pd.get_dummies(dat, columns=["Seasons"])
del dat['Seasons_Winter']
dat = pd.get_dummies(dat, columns=["Holiday"])
del dat['Holiday_Holiday']
dat = pd.get_dummies(dat, columns=["FunctionalDay"])
del dat['FunctionalDay_Yes']
dat.shape
```

[20]:
```
(8760, 16)
```

[4]:
```
dat.head(2)
```

[4]:
```
         Date  RentedBikeCount  Hour  Temp  Humidity  WindSpeed  Visibility  \
0  01/12/2017              254   0.0  -5.2      37.0        2.2      2000.0
1  01/12/2017              204   1.0  -5.5      38.0        0.8      2000.0

   DewPointTemp  SolarRadiation  Rainfall  Snowfall  Seasons_Autumn  \
0         -17.6             0.0       0.0       0.0               0
1         -17.6             0.0       0.0       0.0               0

   Seasons_Spring  Seasons_Summer  Holiday_No Holiday  FunctionalDay_No
0               0               0                   1                 0
```

```
1                0                0                1                0
```

[5]:
```
# split data into X and y
X = dat.iloc[:, 2:dat.shape[1]]
Y = dat.iloc[:,1]
print(f"X size {X.shape} and Y size {Y.shape}")
```

```
X size (8760, 14) and Y size (8760,)
```

3 Model Assuming Independent Observations

- Training and Testing data are selected randomly across the year.
- The 'Date" information is not used.

[6]:
```
# split data into train and test sets
seed = 7
test_size = 0.25
X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size=test_size,␣
 ↪random_state=seed)
```

[7]:
```
print(f"X_train size {X_train.shape}; y_train size {y_train.shape}")
```

```
X_train size (6570, 14); y_train size (6570,)
```

[8]:
```
print(f"X_test size {X_test.shape}; y_test size {y_test.shape}")
```

```
X_test size (2190, 14); y_test size (2190,)
```

3.1 Simple XGBoost Model

- To start with, simply train the model with all training set from previous splitting.
- The training set prediction accuracy reaches 99.997 % but testing accuracy is at 85.487 %.
- The testing ressult is not improving after several iterations.
- The next step is to add CV and tune some parameters

[45]:
```
%%capture
# fit model with training data
start_time = time.time()
model1 = xgb.XGBRegressor(n_estimators=1000)
model1.fit(X_train, y_train,
           eval_set=[(X_train, y_train), (X_test, y_test)],
           verbose=True)
```

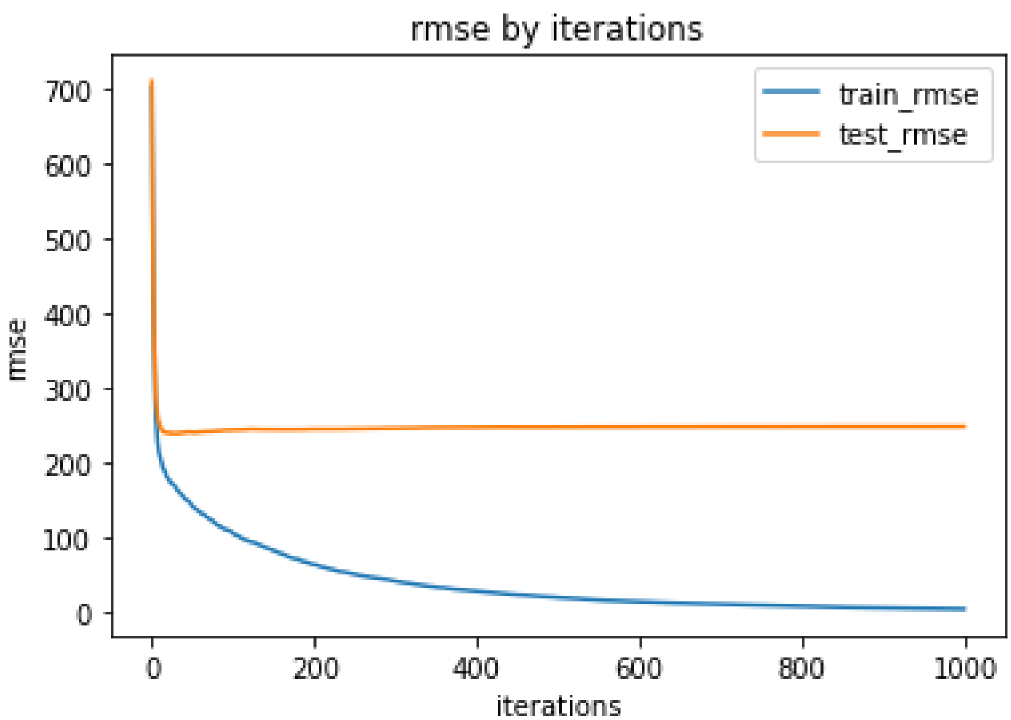
[46]:
```
print(f"Model running for {(time.time()-start_time)/60:0.2f} min.")
```

```
Model running for 0.04 min.
```

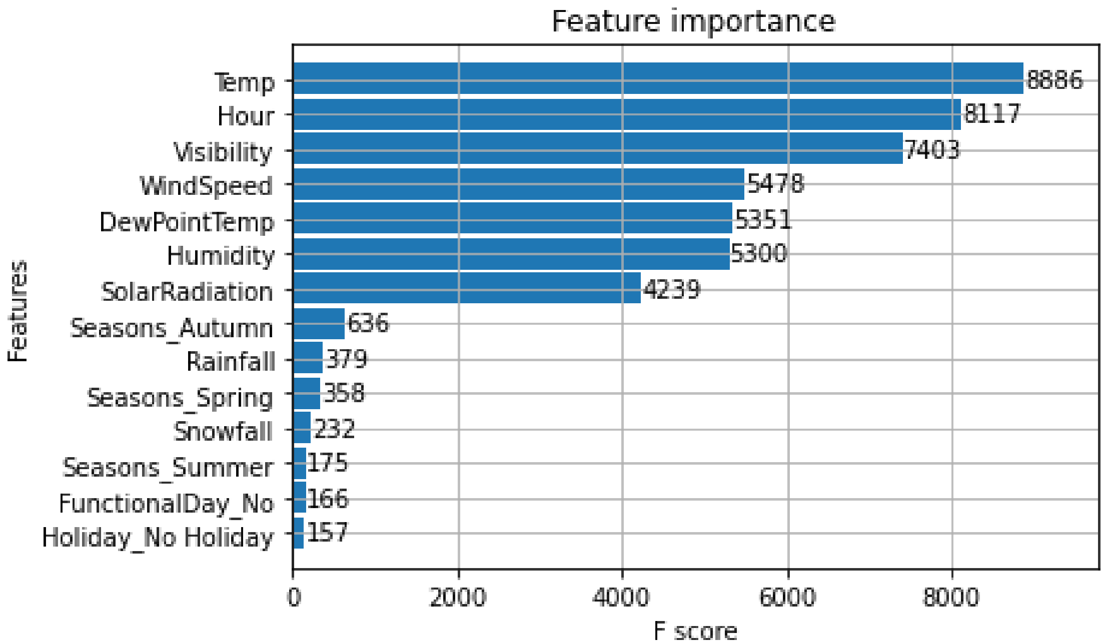
[47]:
```
evals_result1 = model1.evals_result()
```

[48]:
```
def plot_validation(evals_result, metric='rmse', ax=None, title=None):
    train_rmse = evals_result['validation_0'][metric]
    test_rmse = evals_result['validation_1'][metric]
    plot_dat = pd.DataFrame({'train_rmse': train_rmse,
                            'test_rmse': test_rmse})
    title = f"{metric} by iterations" if title is None else title
    plot_dat.plot(xlabel="iterations", ylabel=metric, ax=ax, title=title)
```

[49]:
```
plot_validation(evals_result1)
```



[232]:
```
_ = xgb.plot_importance(model1, height=0.9)
```



[145]:
```
score = model1.score(X_train, y_train)
print(f"Training score: {score*100:.3f} %")
```

```
Training score: 99.997 %
```

[146]:
```
score = model1.score(X_test, y_test)
print(f"Testing score: {score*100:.3f} %")
```

```
Testing score: 85.487 %
```

3.2 Model with GridSearchCV

[35]:
```
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import GridSearchCV
```

[279]:
```
%%capture
start_time = time.time()
parameters = {'nthread':[4], #when use hyperthread, xgboost may become slower
              'objective':['reg:squarederror'],
              'learning_rate': [.03, .07, 0.3], #so called `eta` value
              'max_depth': [3, 5, 7],
              'min_child_weight': [4],
              'silent': [1],
              'subsample': [0.7],
              'colsample_bytree': [0.7],
```

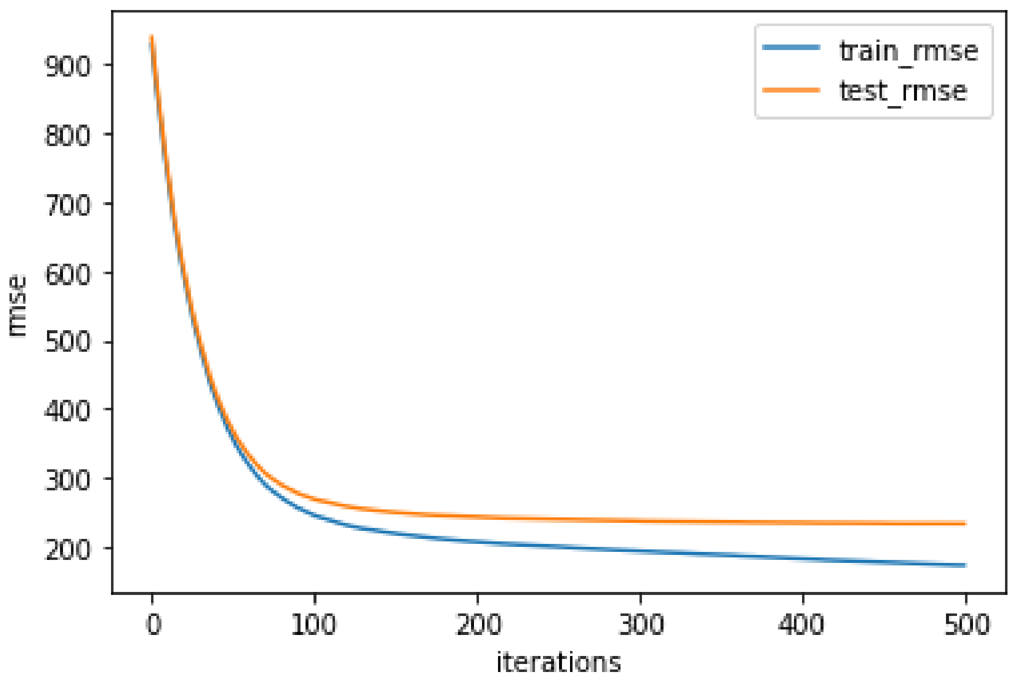
```
             'n_estimators': [500]}

xgb_grid = GridSearchCV(xgb.XGBRegressor(),
                        parameters,
                        cv = 10,
                        n_jobs = 5,
                        verbose=True)
model2 = xgb_grid.fit(X_train, y_train,
                      eval_set=[(X_train, y_train), (X_test, y_test)],
                      verbose=True)
model2 = model2.best_estimator_
```

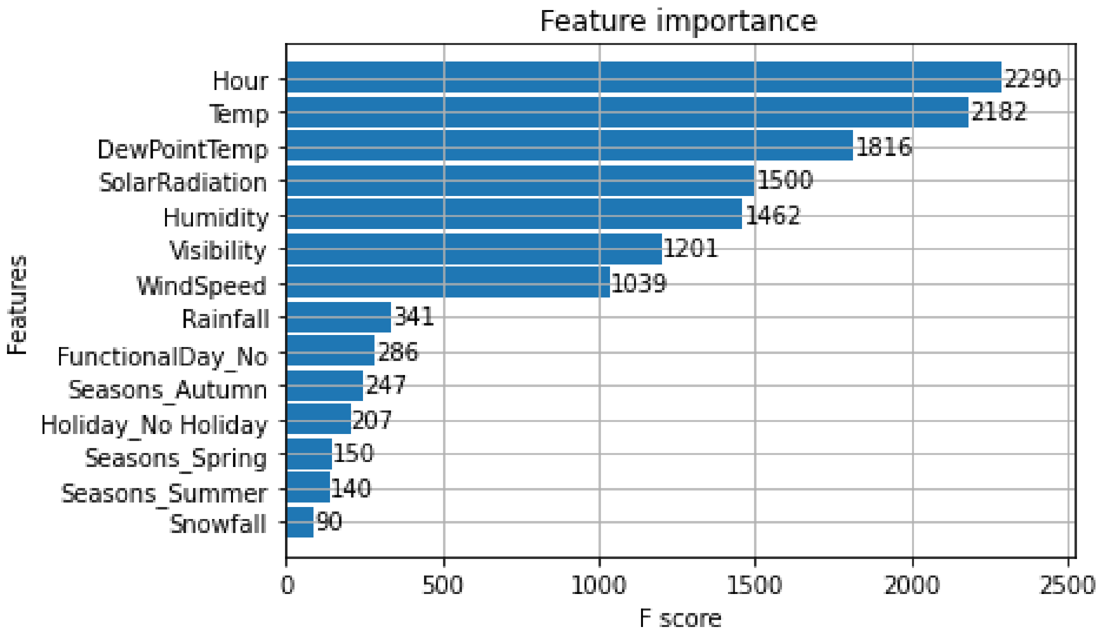
[284]:
```
print(f"Model running for {(time.time()-start_time)/60:0.2f} min.")
```

```
Model running for 2.48 min.
```

[285]:
```
evals_result2 = model2.evals_result()
plot_validation(evals_result2)
```



[286]:
```
_ = xgb.plot_importance(model2, height=0.9)
```



[287]:
```
score = model2.score(X_train, y_train)
print(f"Training score: {score*100:.3f} %")
```

```
Training score: 92.766 %
```

[288]:
```
score = xgb_grid.cv_results_['mean_test_score'].mean()
print(f"CV mean test score: {score*100:.3f} %")
```

```
CV mean test score: 86.589 %
```

[289]:
```
score = model2.score(X_test, y_test)
print(f"Testing score: {score*100:.3f} %")
```

```
Testing score: 87.148 %
```

4 Model Tested with Anchor Date

- In this time series data, an anchor date is defined to split training and testing data.
- The model is trained based on data before anchor date and used to predict observations after anchor date to evaluate accuracy.
- Time series attribution is not included in this model.
- The testing results show:
  - In general lower accuracy compared with random testing data selection
  - The training data lacks information for season Autumn.

- Non-function day attibute is not applied well based on prediction comparison plots. Non-function day record appears mainly during months 9, 10 and 11. Therefore, testing month 11 has the best prediction accuracy as month 9 and 10 information is included in training data.

4.1 Training & Testing Data Splitting with Anchor Date

- In this time series data, observations are based by hour and date.
- 25% testing data equals to around 91 days or 3 months.
- Split the data into 3 sets of training and testing data.

[21]:
```
dat['Date'] = pd.to_datetime(dat['Date'], format="%d/%m/%Y")
```

[25]:
```
dat['Date'].dt.month.unique()
```

[25]:
```
array([12,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11])
```

[115]:
```
dat_set = {}

for test_month in [9, 10, 11]:
    train_dat = dat[(dat['Date'].dt.month < test_month)|(dat['Date'].dt.year ==␣
 ↪2017)]
    test_dat = dat[dat['Date'].dt.month == test_month]
    print(f"Training Data Size {train_dat.shape}; Testing Data Size {test_dat.
 ↪shape}")
    sub_X_train = train_dat.iloc[:, 2:train_dat.shape[1]]
    sub_Y_train = train_dat.iloc[:,1]
    sub_X_test = test_dat.iloc[:, 2:test_dat.shape[1]]
    sub_Y_test = test_dat.iloc[:,1]
    dat_set[test_month] = (sub_X_train, sub_Y_train, sub_X_test, sub_Y_test)
```

```
Training Data Size (6576, 16); Testing Data Size (720, 16)
Training Data Size (7296, 16); Testing Data Size (744, 16)
Training Data Size (8040, 16); Testing Data Size (720, 16)
```

4.2 Model Training and Testing

[97]:
```
def cv_xgb_train(X_training, Y_training, X_testing, Y_testing):
    param = {'nthread':[4], #when use hyperthread, xgboost may become slower
              'objective':['reg:squarederror'],
              'learning_rate': [.03, .07, 0.3], #so called `eta` value
              'max_depth': [3, 5, 7],
              'min_child_weight': [4],
              'silent': [1],
              'subsample': [0.7],
              'colsample_bytree': [0.7],
```

```
                  'n_estimators': [500]}

    x_g = GridSearchCV(xgb.XGBRegressor(),
                       param,
                       cv = 10,
                       n_jobs = 5,
                       verbose=True)
    mod = x_g.fit(X_training,
                  Y_training,
                  eval_set=[(X_training, Y_training), (X_testing, Y_testing)],
                  verbose=True)
    mod = mod.best_estimator_
    return mod, x_g
```

[98]:
```
%%capture
start_time = time.time()
res_summary = {}
res_mod = {}
for k, v in dat_set.items():
    sub_X_train, sub_Y_train, sub_X_test, sub_Y_test = v
    fit_mod, trained_grid = cv_xgb_train(sub_X_train, sub_Y_train, sub_X_test,␣
 ↪sub_Y_test)
    # track mod
    res_mod[k] = fit_mod
    # track metric
    res_summary[k] = {}
    res_summary[k]['train_score'] = fit_mod.score(sub_X_train, sub_Y_train)
    res_summary[k]['mean_cv_score'] = trained_grid.
 ↪cv_results_['mean_test_score'].mean()
    res_summary[k]['test_score'] = fit_mod.score(sub_X_test, sub_Y_test)
```

[100]:
```
print(f"Model running for {(time.time()-start_time)/60:0.2f} min.")
```

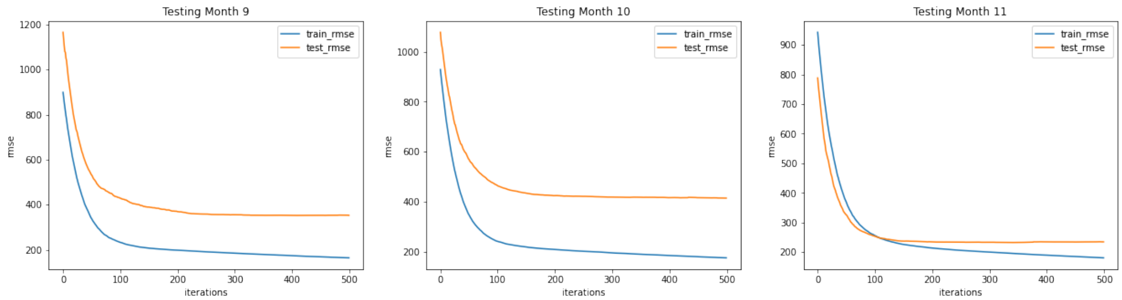
```
Model running for 7.92 min.
```

[99]:
```
pd.DataFrame.from_dict(res_summary)
```

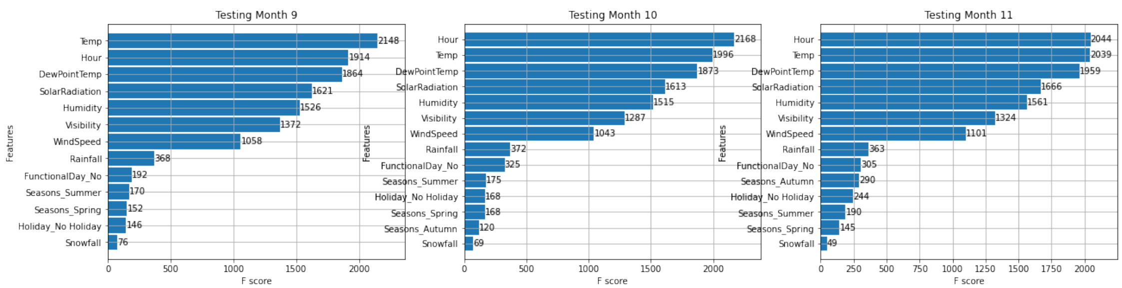
[99]:

	9	10	11
train_score	0.933605	0.928365	0.924187
mean_cv_score	0.624540	0.628203	0.622360
test_score	0.775022	0.606972	0.763277

[101]:
```
fig, ax = plt.subplots(nrows=1, ncols=3, figsize=(21,5))
for k, mod in res_mod.items():
    evals_res = mod.evals_result()
    plot_validation(evals_res, metric='rmse', ax=ax[k-9], title=f"Testing Month␣
 ↪{k}")
```



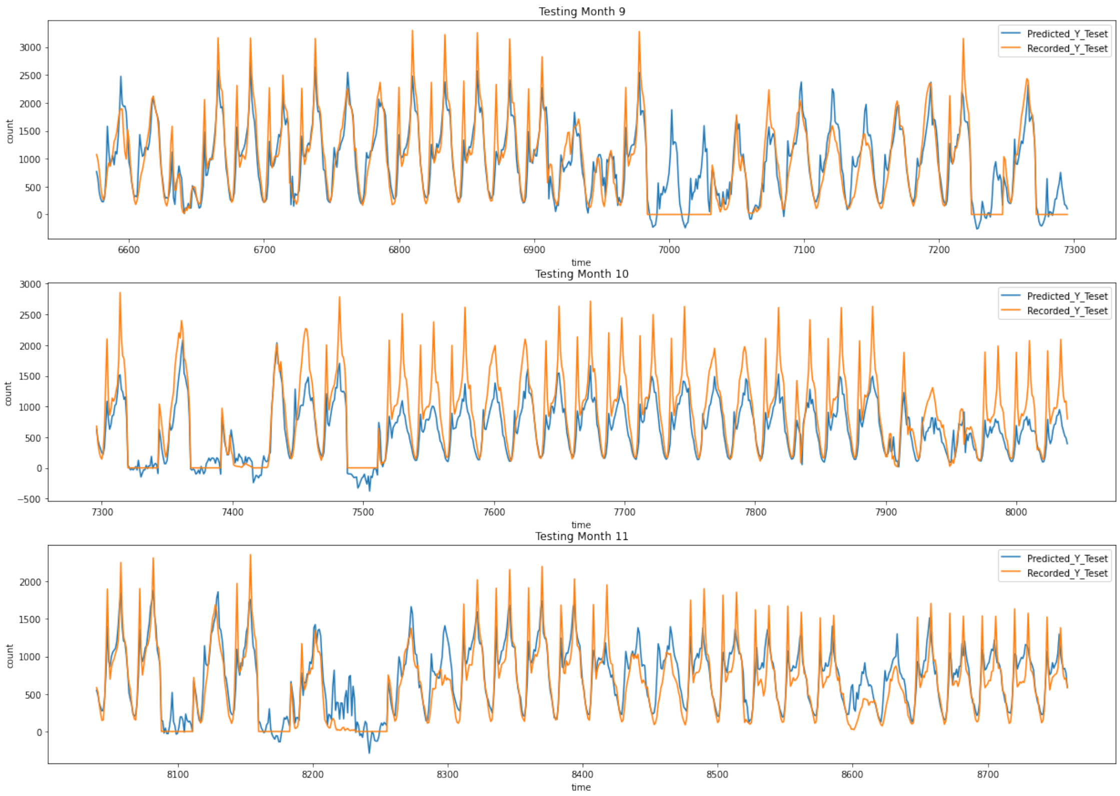

```
[102]: fig, ax = plt.subplots(nrows=1, ncols=3, figsize=(21,5))
for k, mod in res_mod.items():
    xgb.plot_importance(mod, height=0.9, ax=ax[k-9], title=f"Testing Month {k}")
```



4.3 Prediction Accuracy by Time

```
[107]: def plot_prediction(mod, sub_X_test, sub_Y_test, ax=None, title=None):
    y_pred = mod.predict(sub_X_test)
    plot_dat = pd.DataFrame({"Predicted_Y_Teset":y_pred,
                             "Recorded_Y_Teset": sub_Y_test})
    plot_dat.plot(xlabel="time", ylabel="count", ax=ax, title=title)
```

```
[118]: fig, ax = plt.subplots(nrows=3, ncols=1, figsize=(21,15))
for k, mod in res_mod.items():
    sub_X_train, sub_Y_train, sub_X_test, sub_Y_test = dat_set[k]
    plot_prediction(mod, sub_X_test, sub_Y_test, ax=ax[k-9], title=f"Testing␣
↪Month {k}")
```



4.4 Non-function Days

The plots above show a bad prediction on non-function days in month 9. By checking the non-function days across overall data: * 2 days before September 2018 * 4 days in September 2018 * 4 days in October 2018 * 3 days in November 2018

[138]:
```
dat.groupby('FunctionalDay_No').agg({'Date':'nunique'})
```

[138]:

FunctionalDay_No	Date
0	353
1	13

[139]:
```
dat[dat['FunctionalDay_No']==1]['Date'].unique()
```

[139]:
```
array(['2018-04-11T00:00:00.000000000', '2018-05-10T00:00:00.000000000',
       '2018-09-18T00:00:00.000000000', '2018-09-19T00:00:00.000000000',
       '2018-09-28T00:00:00.000000000', '2018-09-30T00:00:00.000000000',
       '2018-10-02T00:00:00.000000000', '2018-10-04T00:00:00.000000000',
       '2018-10-06T00:00:00.000000000', '2018-10-09T00:00:00.000000000',
       '2018-11-03T00:00:00.000000000', '2018-11-06T00:00:00.000000000',
```

```
'2018-11-09T00:00:00.000000000'], dtype='datetime64[ns]')
```

4.5 Model Detail

[155]:
```
for k, mod in res_mod.items():
    print(f"Testing month {k}: \n{mod}")
```

```
Testing month 9:
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.7, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.03, max_delta_step=0, max_depth=5,
             min_child_weight=4, missing=nan, monotone_constraints='()',
             n_estimators=500, n_jobs=4, nthread=4, num_parallel_tree=1,
             random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1,
             silent=1, subsample=0.7, tree_method='exact',
             validate_parameters=1, verbosity=None)
Testing month 10:
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.7, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.03, max_delta_step=0, max_depth=5,
             min_child_weight=4, missing=nan, monotone_constraints='()',
             n_estimators=500, n_jobs=4, nthread=4, num_parallel_tree=1,
             random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1,
             silent=1, subsample=0.7, tree_method='exact',
             validate_parameters=1, verbosity=None)
Testing month 11:
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.7, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.03, max_delta_step=0, max_depth=5,
             min_child_weight=4, missing=nan, monotone_constraints='()',
             n_estimators=500, n_jobs=4, nthread=4, num_parallel_tree=1,
             random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1,
             silent=1, subsample=0.7, tree_method='exact',
             validate_parameters=1, verbosity=None)
```

5 Model with Time Attributes

- There's some improvements in testing but along with slightly overfitting in training data.
- The added attributes ranked in the mid range in importance plots. Temp and Hour are still the two most important attributes.

[121]:
```
dat2 = dat.copy()
dat2['Year'] = dat2['Date'].dt.year
dat2['Month'] = dat2['Date'].dt.month
dat2['Week'] = dat2['Date'].dt.week
dat2['Day'] = dat2['Date'].dt.day
dat2['DayOfWeek'] = dat2['Date'].dt.dayofweek
```

```
<ipython-input-121-1012b0438a4f>:4: FutureWarning: Series.dt.weekofyear and
Series.dt.week have been deprecated.  Please use Series.dt.isocalendar().week
instead.
  dat2['Week'] = dat2['Date'].dt.week
```

[122]:
```
dat2.head(2)
```

[122]:
```
        Date  RentedBikeCount  Hour  Temp  Humidity  WindSpeed  Visibility  \
0 2017-12-01              254   0.0  -5.2      37.0        2.2      2000.0
1 2017-12-01              204   1.0  -5.5      38.0        0.8      2000.0

   DewPointTemp  SolarRadiation  Rainfall  …  Seasons_Autumn  \
0         -17.6             0.0       0.0  …               0
1         -17.6             0.0       0.0  …               0

   Seasons_Spring  Seasons_Summer  Holiday_No Holiday  FunctionalDay_No  Year  \
0               0               0                   1                 0  2017
1               0               0                   1                 0  2017

   Month  Week  Day  DayOfWeek
0     12    48    1          4
1     12    48    1          4

[2 rows x 21 columns]
```

[123]:
```
dat_set2 = {}

for test_month in [9, 10, 11]:
    train_dat = dat2[(dat2['Date'].dt.month < test_month)|(dat2['Date'].dt.year␣
 ↪== 2017)]
    test_dat = dat2[dat2['Date'].dt.month == test_month]
    print(f"Training Data Size {train_dat.shape}; Testing Data Size {test_dat.
 ↪shape}")
    sub_X_train = train_dat.iloc[:, 2:train_dat.shape[1]]
    sub_Y_train = train_dat.iloc[:,1]
    sub_X_test = test_dat.iloc[:, 2:test_dat.shape[1]]
    sub_Y_test = test_dat.iloc[:,1]
    dat_set2[test_month] = (sub_X_train, sub_Y_train, sub_X_test, sub_Y_test)
```

```
Training Data Size (6576, 21); Testing Data Size (720, 21)
```

```
Training Data Size (7296, 21); Testing Data Size (744, 21)
Training Data Size (8040, 21); Testing Data Size (720, 21)
```

[156]:
```
def cv_xgb_train2(X_training, Y_training, X_testing, Y_testing):
    param = {'nthread':[4], #when use hyperthread, xgboost may become slower
                  'objective':['reg:squarederror'],
                  'learning_rate': [.03, .07, 0.3], #so called `eta` value
                  'max_depth': [3, 5],  # limiting max_depth to avoid␣
↪overfitting
                  'min_child_weight': [4],
                  'silent': [1],
                  'subsample': [0.7],
                  'colsample_bytree': [0.7],
                  'n_estimators': [500]}

    x_g = GridSearchCV(xgb.XGBRegressor(),
                       param,
                       cv = 10,
                       n_jobs = 5,
                       verbose=True)
    mod = x_g.fit(X_training,
                  Y_training,
                  eval_set=[(X_training, Y_training), (X_testing, Y_testing)],
                  verbose=True)
    mod = mod.best_estimator_
    return mod, x_g
```

[157]:
```
%%capture
start_time = time.time()
res_summary2 = {}
res_mod2 = {}
for k, v in dat_set2.items():
    sub_X_train, sub_Y_train, sub_X_test, sub_Y_test = v
    fit_mod, trained_grid = cv_xgb_train2(sub_X_train, sub_Y_train, sub_X_test,␣
↪sub_Y_test)
    # track mod
    res_mod2[k] = fit_mod
    # track metric
    res_summary2[k] = {}
    res_summary2[k]['train_score'] = fit_mod.score(sub_X_train, sub_Y_train)
    res_summary2[k]['mean_cv_score'] = trained_grid.
↪cv_results_['mean_test_score'].mean()
    res_summary2[k]['test_score'] = fit_mod.score(sub_X_test, sub_Y_test)
```

[158]:
```
print(f"Model running for {(time.time()-start_time)/60:0.2f} min.")
```

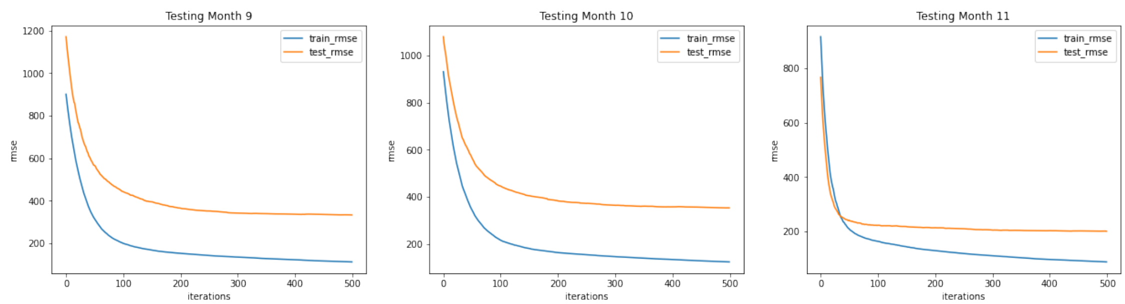
```
Model running for 9.74 min.
```

```
[159]: pd.DataFrame.from_dict(res_summary2)  # TODO check negative values
```

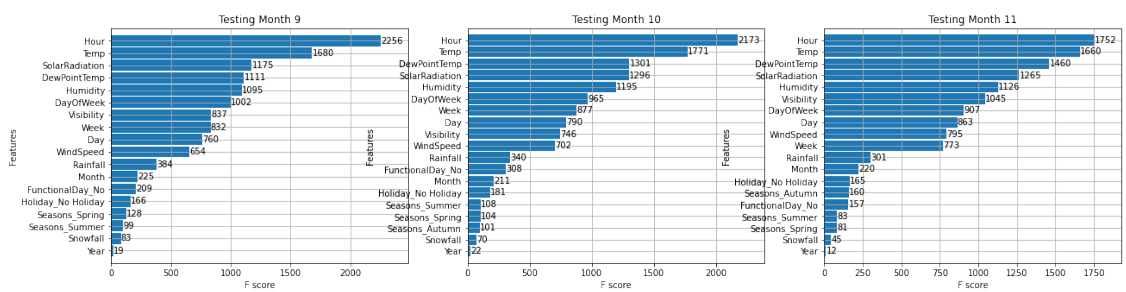
[159]:

	9	10	11
train_score	0.968569	0.964197	0.981632
mean_cv_score	0.687866	0.575854	-0.235344
test_score	0.799063	0.714356	0.825770

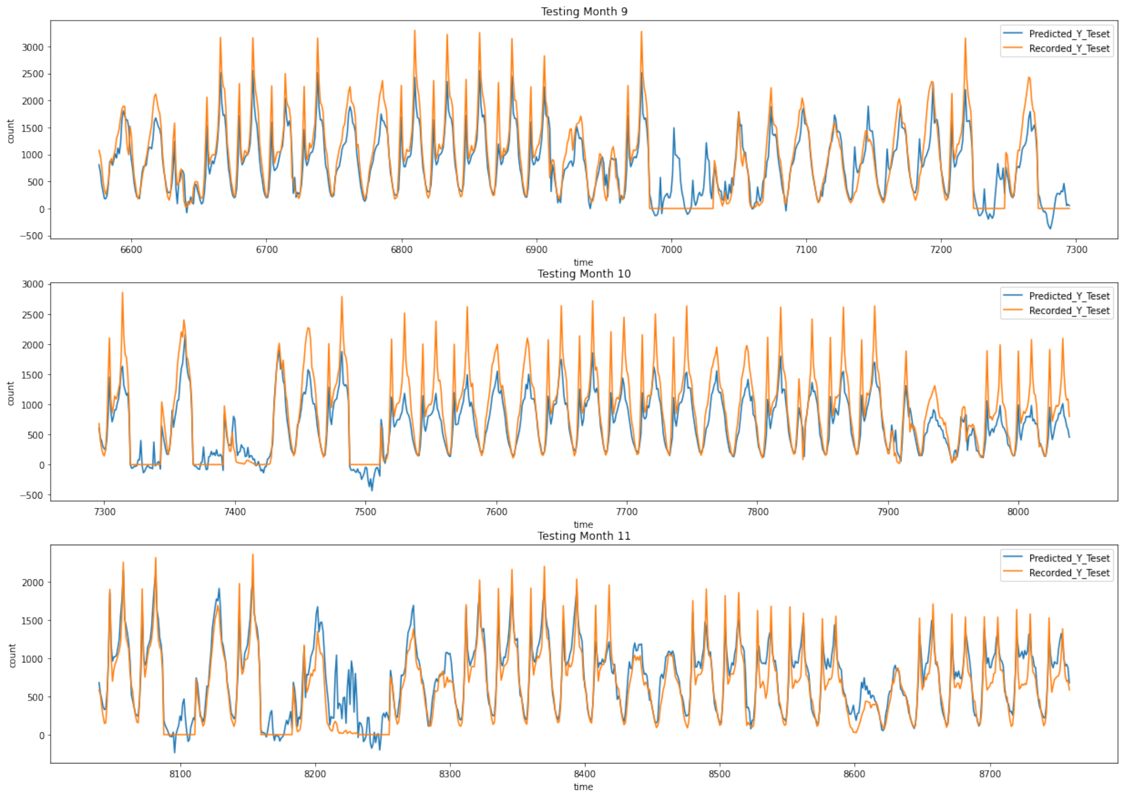
```
[161]: fig, ax = plt.subplots(nrows=1, ncols=3, figsize=(21,5))
       for k, mod in res_mod2.items():
           evals_res = mod.evals_result()
           plot_validation(evals_res, metric='rmse', ax=ax[k-9], title=f"Testing Month {k}")
```




```
[162]: fig, ax = plt.subplots(nrows=1, ncols=3, figsize=(21,5))
       for k, mod in res_mod2.items():
           xgb.plot_importance(mod, height=0.9, ax=ax[k-9], title=f"Testing Month {k}")
```




```
[163]: fig, ax = plt.subplots(nrows=3, ncols=1, figsize=(21,15))
       for k, mod in res_mod2.items():
           sub_X_train, sub_Y_train, sub_X_test, sub_Y_test = dat_set2[k]
           plot_prediction(mod, sub_X_test, sub_Y_test, ax=ax[k-9], title=f"Testing Month {k}")
```



[160]:
```python
for k, mod in res_mod2.items():
    print(f"Testing month {k}: \n{mod}")
```

```
Testing month 9:
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.7, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.03, max_delta_step=0, max_depth=5,
             min_child_weight=4, missing=nan, monotone_constraints='()',
             n_estimators=500, n_jobs=4, nthread=4, num_parallel_tree=1,
             random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1,
             silent=1, subsample=0.7, tree_method='exact',
             validate_parameters=1, verbosity=None)
Testing month 10:
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.7, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.03, max_delta_step=0, max_depth=5,
             min_child_weight=4, missing=nan, monotone_constraints='()',
             n_estimators=500, n_jobs=4, nthread=4, num_parallel_tree=1,
             random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1,
             silent=1, subsample=0.7, tree_method='exact',
```

```
             validate_parameters=1, verbosity=None)
Testing month 11:
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.7, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.07, max_delta_step=0, max_depth=5,
             min_child_weight=4, missing=nan, monotone_constraints='()',
             n_estimators=500, n_jobs=4, nthread=4, num_parallel_tree=1,
             random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1,
             silent=1, subsample=0.7, tree_method='exact',
             validate_parameters=1, verbosity=None)
```