Assignment 1 - Machine Learning

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1 Question 1: Music Taste

We begin with an inspection of the ten most popular artists (defined as artists with the most song plays) and the ten most listened albums (defined as total listeners across all tracks on an album)[1]. Table 1 shows Michael Jackson is by far the most played artist on the radio station, followed by a string of pop and rock artists with 5-7 plays. The column of most popular albums unsurprisingly includes multiple Michael Jackson albums, and further consists of artists who are characterised pretty well by the genres that are also most common in the list of most played artists. In terms of genres, the music taste on the radio station can thus be mostly characterised as having a clear preference for pop and rock.

Table 1: Most Played Artists and Most Listened Songs

Rank	Most Played Artists		Albums with Most Listeners		
	Artist	# Plays	Artist	Album	Listeners
1	Michael Jackson	30	Michael Jackson	Dangerous	231
2	Bryan Adams	7	Michael Jackson	Thriller	203
3	Bruno Mars	6	Savage Garden	Savage Garden	195
4	Coldplay	6	Katy Perry	Teenage Dream	174
5	Placebo	6	Michael Jackson	Bad	157
6	Michael Bolton	6	Amy Winehouse	Back To Black	156
7	Red Hot Chili Peppers	6	Duran Duran	Duran Duran (The Wedding Album)	147
8	The Doors	6	Charlie Puth	Voicenotes	137
9	Aerosmith	5	Cake	Prolonging the Magic	130
10	Duran Duran	5	Spin Doctors	Pocket Full of Kryptonite	129

In terms of quantitative characteristics, we find that the median song played on the radio station can be characterised as being distinctly non-acoustic, non-instrumental yet melody- or beat-heavy (low 'speechiness'), energetic, moderately euphoric (valence) and moderately danceable[2]. Further the median track has a BPM of 120. We would argue this is roughly in line with music recorded by artists shown in table 1, whose music has vocals, is not fully electronic and is neither heavily uplifting nor depressing.

[1]We also considered exhibiting individual songs with the most listeners, but since each song in our dataset is only played once this figure is somewhat arbitrary; the most listened songs might for example simply be those played at the most 'convenient' times.

[2]Of course this statement implicitly assumes that a metric of 0.50 is roughly the median in the Spotify database.

Table 2: Descriptive Statistics

	Mean	SD	Median	Min	Max
artist_popularity	65.71	15.95	68.00	2.00	96.00
album_popularity	52.02	18.77	56.00	0.00	90.00
song_popularity	51.88	20.41	57.00	0.00	98.00
acousticness	0.20	0.24	0.09	0.00	1.00
danceability	0.59	0.14	0.59	0.10	0.98
energy	0.68	0.19	0.71	0.04	0.99
instrumentalness	0.04	0.15	0.00	0.00	0.96
liveness	0.18	0.15	0.12	0.01	0.98
loudness	-7.35	3.11	-6.71	-32.91	-1.36
speechiness	0.05	0.04	0.04	0.02	0.42
tempo	120.25	27.10	117.96	62.51	207.69
valence	0.56	0.24	0.56	0.04	0.99
listener	38.24	17.42	34.00	14.00	81.00

2 Question 2: K-Nearest Neighbors, fixed K

We first decide whether to use a two- or three-way holdout method. Under the latter approach, we would first use the training sample to form a model, and use the validation sample to estimate the model's error. Then we would add our validation sample to our training sample and proceed as the two-way holdout method. In this way, the three way- avoids using our test sample more than once, which is the case in the two-way holdout. This decreases the risk of an optimistic bias in our estimate of the generalization performance. However, it is likely to cause the estimate of the generalization error to be overly pessimistic as the model might not reach its full capacity with the limited amount of training data that remains after splitting the data in a train, validation and test set (Raschka, 2018)[3]. Therefore, we opt to use a two-way holdout approach to evaluate the performance of a K-Nearest Neighbors (KNN) model with $k = 5$.

Afterwards we will compare our MSE with the total number of observations. A relatively large MSE can indicate that our data set indeed is too small to use a three way method. Furthermore, the Mahalanobis distance is used as a measure of distance instead of the standard Euclidean distance[4]. The covariance matrix (whose inverse is used to compute the Mahalanobis distance) is estimated in each fold to make sure that no information is leaked from the test set to the training set, as this differs for each fold.

Six different methods will be used to evaluate the performance of the model specified earlier: the Holdout method, the Repeated holdout method, the Leave-One-Out Cross-Validation (LOOCV) method, the 10-fold Cross-Validation (CV), the Nested 10-fold Cross Validation (N-10-CV) and the bootstrapping method. The choice for 10-folds balances bias, variance and computational efficiency. The value is also quite common in practice (see footnote 3) and is computationally practical for our hardware. In the holdout-, repeated holdout- and bootstrapping methods, we use 80 percent of our data for the fitting process as a training sample, leaving 20 percent of the data for the test sample. We use the mean squared error (MSE) and the mean absolute error (MAE) as error measures. As KNN cannot cope with nominal variables (there is no concept of distance/scale, unless explicitly introduced), we exclude artist name, album name and song name from the data. This leaves us with 1483 observations, the number of listeners as dependent variable and all other numeric variables (12 in total) as independent variables.

In table 3 the results of the KNN with the k can be found for all methods. Note that as the holdout method is the same as the repeated holdout method with iterations equal to one, these methods are in the same graph. The table shows that the MSE for all methods ranges between 338 and 387 listeners, and the MAE for all methods between 15 and 17. The holdout method gives the lowest MSE (though not the lowest

[3]Raschka, S. (2018), *Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning*, url: `https://arxiv.org/abs/1811.12808v2`

[4]The Mahalanobis distance is a generalisation of the Euclidian distance that transforms the probability vector space to rescale the axes to have a unit variance. In this sense, the Euclidean distance is a special case of the Mahalanobis in which the covariance matrix equals the identity.

MAE). However, this might be due to the fact that the holdout method only has one iteration. Hence, it uses the least information. The low MSE can thus be a “lucky shot”. In figure 2a (LOOCV), we see that the MAE and MSE peak when n (number of folds) is very low. This is not a surprising result since the number of folds is equal to the number of observations with this method. When using a very low number of observations, leaving one out greatly influences the composition of the data sample and thus the average MSE and MAE as well. From the graphs we see that if we vary the number of bootstraps, folds or iterations using the bootstrap, 10-CV and repeated holdout method respectively, the MSE and MAE are not influenced a lot. Increasing the number of iterations adds information to the model. However, as the errors do not change much across, this indicates that our model has perhaps reached its capacity to extract information from the dataset with this hyperparameter setting. Further, it is worth noting that for all methods, using either the MSE or the MAE, the test errors are a lot higher than the training errors. This is not surprising, since the training errors give an optimistic estimation of the error measures. The bootstrapped result is highly dependent on the train and test split, as one bootstrapping procedure only splits the data once. As we’ve seen the error is quite sensitive to different splits of the data. Furthermore, graph 2a is shown without the standard errors for the test error, as it is orders of magnitude larger than the standard errors of other evaluation methods, this is to be expected from LOOCV, as the test set is just one observation.

Table 3: Result of KNN with fixed k ($k = 5$)

	MSE		MAE	
Evaluation method	$\hat{\mu}$	$\hat{\sigma}$	$\hat{\mu}$	$\hat{\sigma}$
Holdout	338.2290	-	15.6902	-
Repeated holdout	353.5822	21.1714	15.6367	0.5127
LOOCV	349.0405	4.028×10^2	15.6028	1.0276×10^1
10-fold CV	349.0740	29.1240	15.5627	0.4967
Nested 10-fold CV	351.5136	3.2539	15.6107	0.0880
Bootstrapped	386.5762	20.5983	16.3035	0.4819

Figure 1a: 10-fold CV

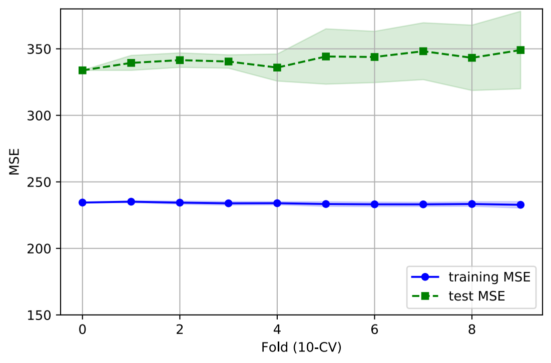


Figure 1b: Nested 10-fold CV

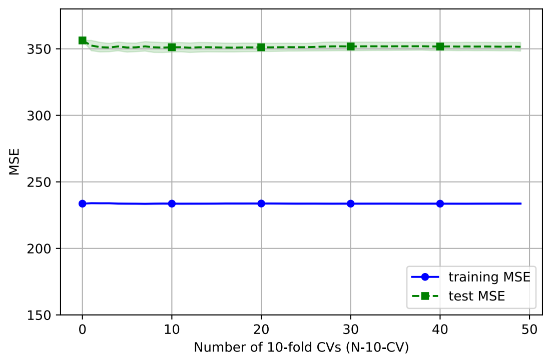


Figure 2a: LOOCV

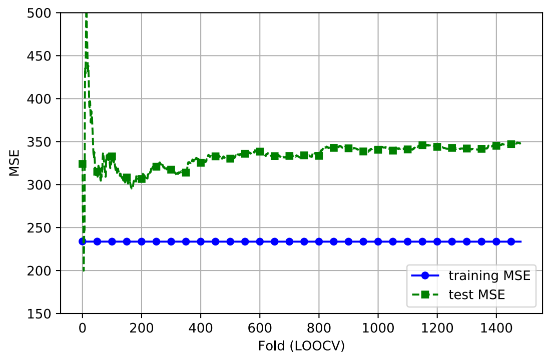
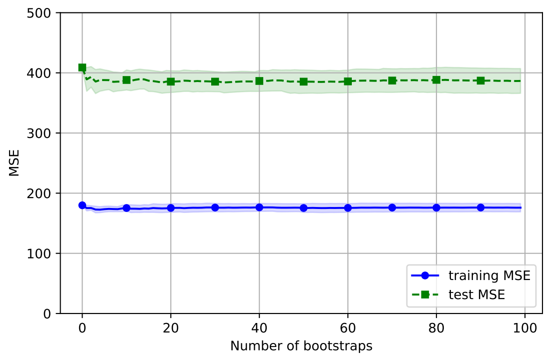


Figure 2b: Bootstrapped



3 Question 3: K-Nearest Neighbors, varying k

In this section we revisit regression based on the KNN model using the same methods as in question 2. However, this time we want to evaluate the error for different values of k as opposed to holding it fixed at $k = 5$.

For the LOOCV we have $n = 1083$ (the number of observations in our training sample). Moreover, we will estimate the model using $k = 1, 2, ..., 20$ for these methods. We set the largest permitted value of k at 20 to limit the computational burden when applying the LOOCV and N-10-CV methods. We again use the MSE and MAE as error measurements. Based on these measurements we can see for which value of k in this range the model performance is optimized. In table 4 the results of the KNN hyperparameter optimization for k can be found for all methods. Figures 3a-3d show the results of the optimization of k using the 10-fold CV-, LOOCV- and bootstrapping methods.

From the graphs we see that for all methods, the larger k, the closer the MSE and MAE of the test and training sample are. Moreover, for all methods we see that the optimal k is the largest permitted value of 20, suggesting that model fit improves when we increase the number of nearest neighbors. This would in turn suggest that there may be further scope for improvement of the predictive performance if we were less concerned with the required computing power (and allowed $k > 20$. We see in table 4 that for all methods the optimal value of k is unequal to 5. Moreover, for all methods but the nested 10-CV, the variance of the MSE has decreased. All in all, model performance has improved. The holdout method is again the outperformer, now in terms of MSE as well as in terms in MAE. In fact, among all methods employed in this paper, the holdout method with $k = 13$ is the only one to achieve a MSE of under 300. This result appears to be a “lucky shot”, as the MSE shoots back up to 311 or 337 when we choose $k = 12$ or $k = 14$ respectively.

For our conclusion about the general performance of our model we see that making k flexible (unsurprisingly) improves model performance. This indicates that our model using the optimal k gives a reasonable accurate prediction of the number of listeners.

Table 4: Results of KNN hyperparameter optimization for k $(1, \ldots, 20)$

	MSE			MAE		
Evaluation method	Optimal K	$\hat{\mu}$	$\hat{\sigma}$	Optimal K	$\hat{\mu}$	$\hat{\sigma}$
Holdout	13	277.7071	-	13	14.2189	-
Repeated holdout	20	303.1302	17.1427	20	14.7356	0.4622
LOOCV	20	302.1827	331.4328	20	14.7424	9.2111
10-fold CV	20	301.6786	23.2308	20	14.7341	0.6161
Nested 10-fold CV	20	301.5956	1.7259	20	14.7269	0.0460
Bootstrapped	20	304.8919	8.3818	20	14.8740	0.2529

Figure 3a: 10-fold CV

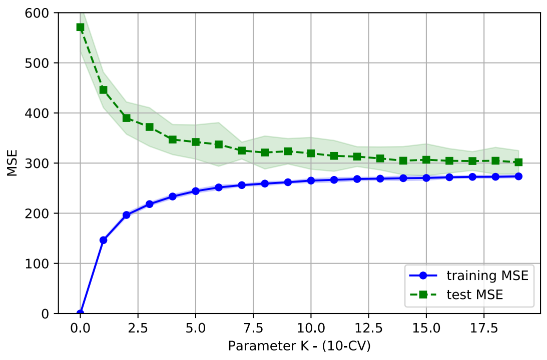


Figure 3b: Nested 10-fold CV

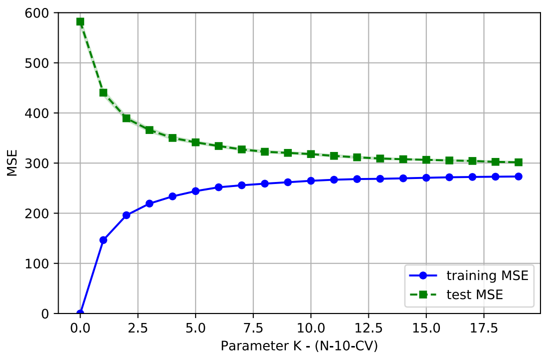


Figure 3c: LOOCV

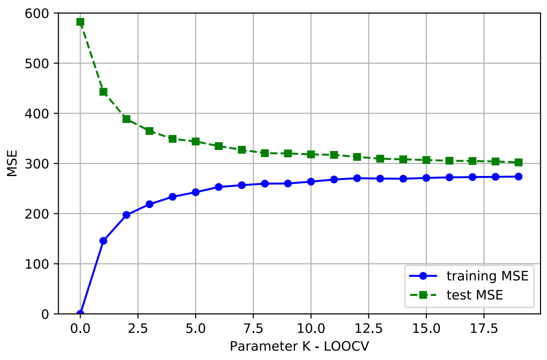


Figure 3d: Bootstrapped

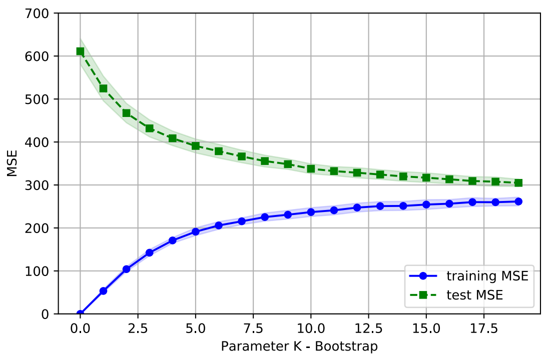
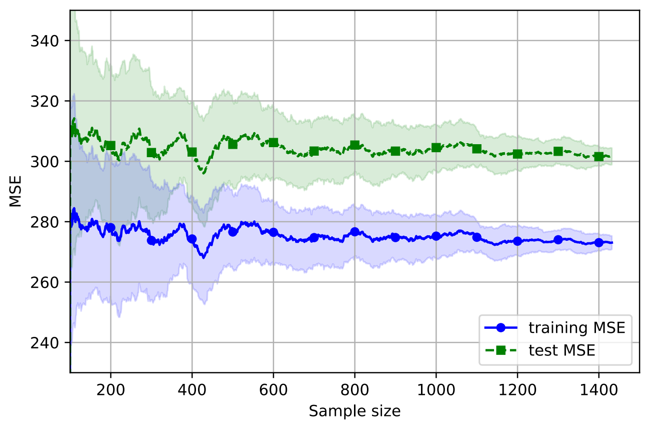


Figure 4 shows the estimated error of the training and test sets with 10-fold CV at different sample sizes and hyperparameter $k = 20$. The figure starts at 50 observations and is a rolling average of the last 50 observations, to compensate for the sensitivity of the error to differences in train and test splits. This is the *learning curve* of our model and dataset. As one can observe, the MSE levels off after a sample size of 1200, for smaller sample sizes it is still improving. We can reasonably argue that the two-way holdout approach was justified; the decreased training sample size that results from using a validation sample in the three-way holdout approach might have negatively affected the MSE.

Figure 4: Learning curve ($k = 20$)



4 Appendix: Python - Jupyter Notebooks

The first notebook is for Question 1. This can be accessed on `https://drive.google.com/open?id=112oKOpZ7qr4vYVDHJKmDyVwSvSCzVARj`

The second notebook is for Questions 2 & 3. This notebook can be accessed on `https://drive.google.com/open?id=1i8QnCBn-Qx5Vf9d2_btVSQGK44n_Xwm1`

Exploratory Statistics

September 16, 2019

1 Setup

[1]:
```
import pandas as pd
import numpy as np
```

1.0.1 Load and view dataset

[11]:
```
data = pd.read_csv('hw2_data.txt', sep='\t')
```

[12]:
```
data.head()
```

[12]:
```
   listener       artist_name                          album_name  \
1        64              P!nk                        Walk Me Home
2        62  Belinda Carlisle  Greatest Vol.1 - Belinda Carlisle
3        61            Travis                         The Man Who
4        51     Freya Ridings                             Castles
5        53      Stephen Puth                         Sexual Vibe

                      song_name  artist_popularity  album_popularity  \
1                  Walk Me Home                 88                77
2      Heaven Is a Place on Earth                65                64
3  Why Does It Always Rain On Me?                63                49
4                       Castles                 69                51
5                   Sexual Vibe                 56                54

   song_popularity  acousticness  danceability  energy  instrumentalness  \
1               86        0.0519         0.652   0.453          0.000000
2               71        0.0243         0.640   0.852          0.000002
3               57        0.0790         0.497   0.537          0.000139
4               60        0.0046         0.672   0.752          0.000470
5               63        0.0191         0.803   0.782          0.000005

   liveness  loudness  speechiness    tempo  valence
1    0.1790    -6.119       0.0445   88.038    0.432
2    0.0497    -8.119       0.0345  122.902    0.793
3    0.0782    -9.264       0.0269  108.448    0.371
```

```
4    0.0560    -4.866       0.0843  116.945    0.429
5    0.1080    -3.873       0.0289  115.028    0.785
```

2 Question 1

2.0.1 Descriptives

[22]:
```
numeric_vars = list(data.columns)[4:]
numeric_vars
```

[22]:
```
['artist_popularity',
 'album_popularity',
 'song_popularity',
 'acousticness',
 'danceability',
 'energy',
 'instrumentalness',
 'liveness',
 'loudness',
 'speechiness',
 'tempo',
 'valence']
```

[30]:
```
cols = ['Mean', 'SD', 'Median', 'Min', 'Max']
descriptives = pd.DataFrame(index = numeric_vars , columns = cols)
```

[32]:
```
for var in numeric_vars:
    descriptives.loc[var, 'Mean'] = data[var].mean()
    descriptives.loc[var, 'SD'] = data[var].std()
    descriptives.loc[var, 'Median'] = data[var].median()
    descriptives.loc[var, 'Min'] = data[var].min()
    descriptives.loc[var, 'Max'] = data[var].max()
```

[39]:
```
descriptives = descriptives.astype(float).round(2)
```

[40]:
```
print(descriptives.to_latex(header=True))
```

```
\begin{tabular}{lrrrrr}
\toprule
{} &    Mean &     SD &  Median &    Min &     Max \\
\midrule
artist\_popularity &   65.71 &  15.95 &   68.00 &   2.00 &   96.00 \\
album\_popularity  &   52.02 &  18.77 &   56.00 &   0.00 &   90.00 \\
song\_popularity   &   51.88 &  20.41 &   57.00 &   0.00 &   98.00 \\
acousticness      &    0.20 &   0.24 &    0.09 &   0.00 &    1.00 \\
danceability      &    0.59 &   0.14 &    0.59 &   0.10 &    0.98 \\
energy            &    0.68 &   0.19 &    0.71 &   0.04 &    0.99 \\
instrumentalness  &    0.04 &   0.15 &    0.00 &   0.00 &    0.96 \\
liveness          &    0.18 &   0.15 &    0.12 &   0.01 &    0.98 \\
loudness          &   -7.35 &   3.11 &   -6.71 & -32.91 &   -1.36 \\
speechiness       &    0.05 &   0.04 &    0.04 &   0.02 &    0.42 \\
tempo             &  120.25 &  27.10 &  117.96 &  62.51 &  207.69 \\
valence           &    0.56 &   0.24 &    0.56 &   0.04 &    0.99 \\
\bottomrule
\end{tabular}
```

2.0.2 Correlations

[55]:
```
popularity_data = data[['listener', 'artist_popularity', 'album_popularity',␣
 ↪'song_popularity']]
print(popularity_data.corr().round(2).to_latex(header=True))
```

```
\begin{tabular}{lrrrr}
\toprule
{} &  listener &  artist\_popularity &  album\_popularity &  song\_popularity \\
\midrule
listener           &      1.00 &               0.06 &              0.05 &
0.06 \\
artist\_popularity &      0.06 &               1.00 &              0.72 &
0.65 \\
album\_popularity  &      0.05 &               0.72 &              1.00 &
0.91 \\
song\_popularity   &      0.06 &               0.65 &              0.91 &
1.00 \\
\bottomrule
\end{tabular}
```

2.0.3 Most popular artists and songs

[167]:
```
# Group songs by artist and name (prevent issues due to same song names for␣
 ↪different artists), find most listened
most_played_songs = data.groupby(['artist_name', 'song_name'])['listener'].
 ↪sum().sort_values(ascending=False)[:10]
```

[180]:
```
# Group songs by artists, find most played artists
most_played_artists = (data.groupby(['artist_name'])['listener']
                       .count()
                       .sort_values(ascending=False)[:10]
```

```
                        .reset_index()
                        .rename(columns = {'listener' : 'songs_played'}))

most_played_artists.index += 1 # start index counting at 1 (ranks 1-10 instead␣
↪of 0-9)
```

[181]:
```
most_listened_albums = (data.groupby(['artist_name', 'album_name'])['listener']
                         .sum()
                         .sort_values(ascending=False)[:10]
                         .reset_index())

most_listened_albums.index += 1
```

[183]:
```
most_listened_albums
```

[183]:
```
       artist_name                                        album_name  \
1   Michael Jackson                                         Dangerous
2   Michael Jackson                    Thriller 25 Super Deluxe Edition
3     Savage Garden                                     Savage Garden
4        Katy Perry  Katy Perry - Teenage Dream: The Complete Confe…
5   Michael Jackson                             Bad 25th Anniversary
6     Amy Winehouse                                     Back To Black
7       Duran Duran                     Duran Duran [The Wedding Album]
8      Charlie Puth                                        Voicenotes
9              Cake                              Prolonging the Magic
10     Spin Doctors                          Pocket Full Of Kryptonite

    listener
1        231
2        203
3        195
4        174
5        157
6        156
7        147
8        139
9        130
10       129
```

[182]:
```
print(pd.concat([most_played_artists, most_listened_albums], axis=1).
↪to_latex(header=True))
```

```
\begin{tabular}{llrllr}
\toprule
{} &            artist\_name &  songs\_played &      artist\_name &
album\_name &  listener \\
\midrule
```

```
1  &        Michael Jackson &            30 &  Michael Jackson &
Dangerous &       231 \\
2  &            Bryan Adams &             7 &  Michael Jackson &
Thriller 25 Super Deluxe Edition &       203 \\
3  &             Bruno Mars &             6 &    Savage Garden &
Savage Garden &       195 \\
4  &               Coldplay &             6 &       Katy Perry &  Katy Perry -
Teenage Dream: The Complete Confe… &       174 \\
5  &                Placebo &             6 &  Michael Jackson &
Bad 25th Anniversary &       157 \\
6  &         Michael Bolton &             6 &    Amy Winehouse &
Back To Black &       156 \\
7  &  Red Hot Chili Peppers &             6 &      Duran Duran &
Duran Duran [The Wedding Album] &       147 \\
8  &              The Doors &             6 &     Charlie Puth &
Voicenotes &       139 \\
9  &              Aerosmith &             5 &             Cake &
Prolonging the Magic &       130 \\
10 &            Duran Duran &             5 &     Spin Doctors &
Pocket Full Of Kryptonite &       129 \\
\bottomrule
\end{tabular}
```

3 Question 2

[158]:
```
data.groupby(['artist_name', 'song_name'])['listener'].sum().
↪sort_values(ascending=False)[:10]
```

[158]:
```
artist_name                song_name
Bon Jovi                   Have A Nice Day               81
The Cranberries            Animal Instinct               80
Suede                      Beautiful Ones (Remastered)   79
Louis Tomlinson            Two of Us                     79
kent                       Music Non Stop                79
EMF                        Unbelievable                  78
Lisa Loeb & Nine Stories   Do You Sleep?                 78
Sunrise Avenue             Lifesaver                     77
Christina Aguilera         Genie in a Bottle             77
Michael Bublé              It's a Beautiful Day          77
Name: listener, dtype: int64
```

[ ]:

ML1

September 16, 2019

```
[1]: import numpy as np
     import pandas as pd
     import matplotlib.pyplot as plt
```

```
[2]: data = pd.read_csv('./data/hw2_data.txt', sep='\t')
```

```
[148]: # #Dump all environment variables
       #import dill
       #dill.dump_session('notebook_env.db')
```

```
[3]: #Import all environment variables
     import dill
     dill.load_session('notebook_env.db')
```

```
[3]: from sklearn.model_selection import train_test_split, KFold
     from sklearn.neighbors import KNeighborsRegressor

     data = pd.read_csv('./data/hw2_data.txt', sep='\t')
     X, y = data.iloc[:,4:].to_numpy(), data.iloc[:,0].to_numpy()

     test_size = 0.2
```

```
[6]: #Error measures

     def MSE(true, pred):
         MSE = np.mean((true-np.round(pred))**2)
         return MSE

     def MAE(true, pred):
         MAE = np.mean(np.abs(true-np.round(pred)))
         return MAE
```

1 Question 2 (K=5), fixed K

[7]:
```
n_neighbors = 5
```

1.1 Holdout

[8]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=test_size,
                                                    random_state=1)
V = np.cov(X_train.T)

KNN_regressor = KNeighborsRegressor(n_neighbors=n_neighbors,
                                    weights='uniform',
                                    algorithm='auto',
                                    metric='mahalanobis',
                                    metric_params={'V':V})

KNN_regressor.fit(X_train, y_train)
pred = KNN_regressor.predict(X_test)

print(f" Holdout \n MSE: {MSE(y_test, pred):.4f}\n MAE: {MAE(y_test, pred):.
 ↪4f}" )

# %store X_train
# %store X_test
# %store y_train
# %store y_test
```

```
 Holdout
 MSE: 338.2290
 MAE: 15.6902
```

1.2 Repeated holdout

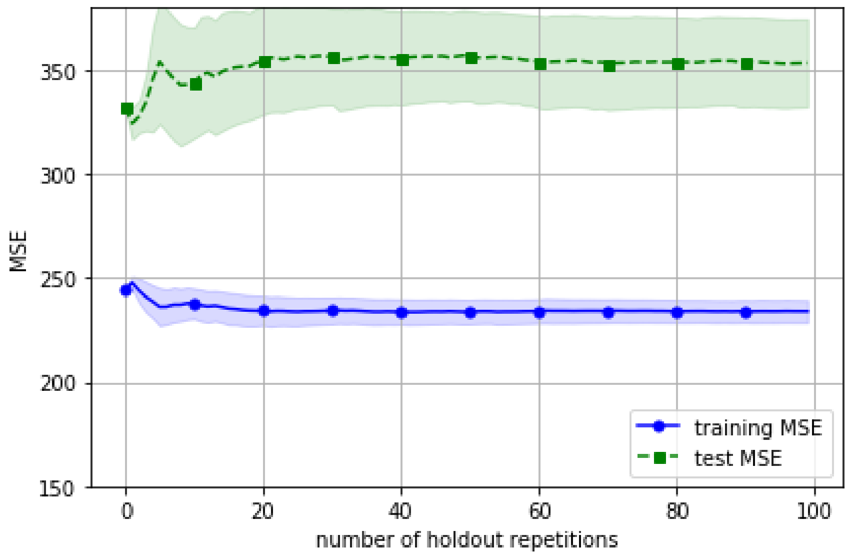
[9]:
```
def repeated_holdout(X, y, n, test_size, n_neighbors, seed=12345, log=True):

    rng = np.random.RandomState(seed=seed)
    seeds = np.arange(10**5); rng.shuffle(seeds)
    seeds=seeds[:n]

    metrics, means, std = [np.empty((n,4)) for _ in range(3)]

    for index, seed in enumerate(seeds):
        X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                        test_size=test_size,
                                                        random_state=seed)
        V = np.cov(X_train.T)

        KNN_regressor = KNeighborsRegressor(n_neighbors=n_neighbors,
                                            weights='uniform',
                                            algorithm='auto',
                                            metric='mahalanobis',
                                            metric_params={'V':V})

        KNN_regressor.fit(X_train, y_train)
        pred_test = KNN_regressor.predict(X_test)
        pred_train = KNN_regressor.predict(X_train)
        metrics[index,:] = MSE(y_test, pred_test), MAE(y_test, pred_test),␣
↪MSE(y_train, pred_train), MAE(y_train, pred_train)
        means[index,:] = np.mean(metrics[:(index+1)], axis=0)
        std[index,:] = np.std(metrics[:(index+1)], axis=0)

        if ((index+1) % (int(n/10)) == 0) & log:
            print(f"{index+1} / {n} test MSE: {metrics[index,:][0]:.4f} std:␣
↪{std[index,:][0]:.4f} | train MSE: {metrics[index,:][2]:.4f} std:␣
↪{std[index,:][2]:.4f}")
    if log:
        print("Done!")

    return metrics, means, std
```

```
[10]: def plot_train_test(train_mean, train_std, test_mean, test_std, length,␣
↪markevery, xlab, ylab, lim, file, std=True):

    number_of_repetitions = np.arange(length)

    plt.plot(number_of_repetitions, train_mean,
             color='blue', marker='o',
             markersize=5, label=f'training {ylab}', markevery=markevery)

    plt.plot(number_of_repetitions, test_mean,
             color='green', linestyle='--',
             marker='s', markersize=5,
             label=f'test {ylab}', markevery=markevery)

    if std:
        plt.fill_between(number_of_repetitions,
                         test_mean + test_std,
                         test_mean - test_std,
                         alpha=0.15, color='green')
        plt.fill_between(number_of_repetitions,
                         train_mean + train_std,
                         train_mean - train_std,
                         alpha=0.15, color='blue')

    plt.grid()
    plt.xlabel(f'{xlab}')
    plt.ylabel(f'{ylab}')
    plt.legend(loc='lower right')
    plt.ylim(lim)
    plt.tight_layout()
    plt.savefig(f'images/{file}.svg', dpi=300)
    plt.show()
```

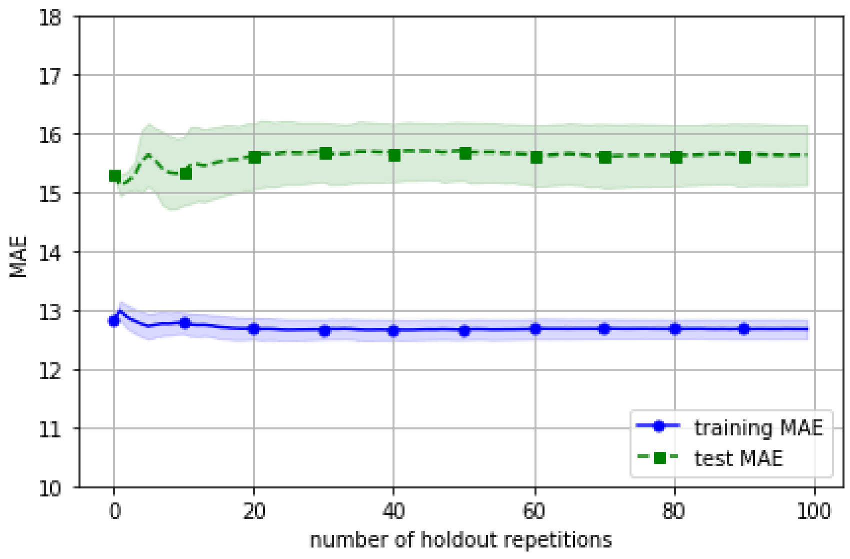
[11]:
```
n = 100

metrics_rh, means_rh, std_rh = repeated_holdout(X, y, n, test_size, n_neighbors)
```

```
10 / 100 test MSE: 345.0303 std: 27.7801 | train MSE: 243.7462 std: 7.7128
20 / 100 test MSE: 384.8182 std: 26.2690 | train MSE: 232.6400 std: 7.3160
30 / 100 test MSE: 352.9529 std: 23.5281 | train MSE: 238.1737 std: 6.4456
40 / 100 test MSE: 365.3973 std: 22.6153 | train MSE: 229.6788 std: 6.1511
50 / 100 test MSE: 379.4209 std: 21.7601 | train MSE: 228.3685 std: 5.8853
60 / 100 test MSE: 341.6902 std: 21.8556 | train MSE: 236.8879 std: 5.8212
70 / 100 test MSE: 374.5084 std: 22.3327 | train MSE: 232.4840 std: 5.7130
80 / 100 test MSE: 356.7980 std: 21.7454 | train MSE: 228.5261 std: 5.5356
90 / 100 test MSE: 307.6296 std: 21.6647 | train MSE: 241.7960 std: 5.4856
100 / 100 test MSE: 361.6869 std: 21.1714 | train MSE: 231.9890 std: 5.4370
Done!
```

[12]:
```
train_mean = means_rh[:,2]
train_std = std_rh[:,2]
test_mean = means_rh[:,0]
test_std = std_rh[:,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=n,
                markevery=10,
                xlab='number of holdout repetitions',
                ylab='MSE',
                lim=[150, 380],
                file='MSE_holdout100')
```



```
[13]: train_mean = means_rh[:,3]
      train_std = std_rh[:,3]
      test_mean = means_rh[:,1]
      test_std = std_rh[:,1]

      plot_train_test(train_mean,
                      train_std,
                      test_mean,
                      test_std,
                      length=n,
                      markevery=10,
                      xlab='number of holdout repetitions',
                      ylab='MAE',
                      lim=[10, 18],
                      file='MAE_holdout100')
```



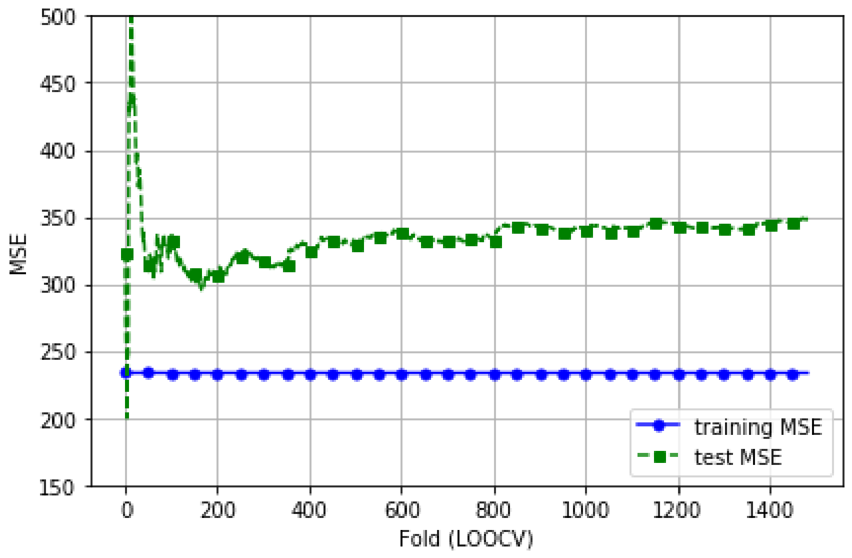
1.3 Leave-One-Out Cross-Validation (LOOCV)

[14]:
```
def loocv(X, y, n_neighbors, log=True, seed=1):

    n = X.shape[0]

    metrics, means, std = [np.empty((n,4)) for _ in range(3)]

    cv = KFold(n_splits=n, shuffle=True, random_state=seed)

    for index, (train_index, test_index) in enumerate(cv.split(X, y)):

        V = np.cov(X[train_index].T)

        KNN_regressor = KNeighborsRegressor(n_neighbors=n_neighbors,
                                             weights='uniform',
                                             algorithm='auto',
                                             metric='mahalanobis',
                                             metric_params={'V':V})

        KNN_regressor.fit(X[train_index], y[train_index])
        pred_test = KNN_regressor.predict(X[test_index])
        pred_train = KNN_regressor.predict(X[train_index])
        metrics[index,:] = MSE(y[test_index], pred_test), MAE(y[test_index],␣
↪pred_test), MSE(y[train_index], pred_train), MAE(y[train_index], pred_train)
        means[index,:] = np.mean(metrics[:(index+1)], axis=0)
        std[index,:] = np.std(metrics[:(index+1)], axis=0)

        if ((index+1) % (int(n/10)) == 0) & log:
            print(f"{index+1} / {n} test MSE: {metrics[index,:][0]:.4f} std:␣
↪{std[index,:][0]:.4f} | train MSE: {metrics[index,:][2]:.4f} std:␣
↪{std[index,:][2]:.4f}")
    if log:
        print("Done!")

    return metrics, means, std
```

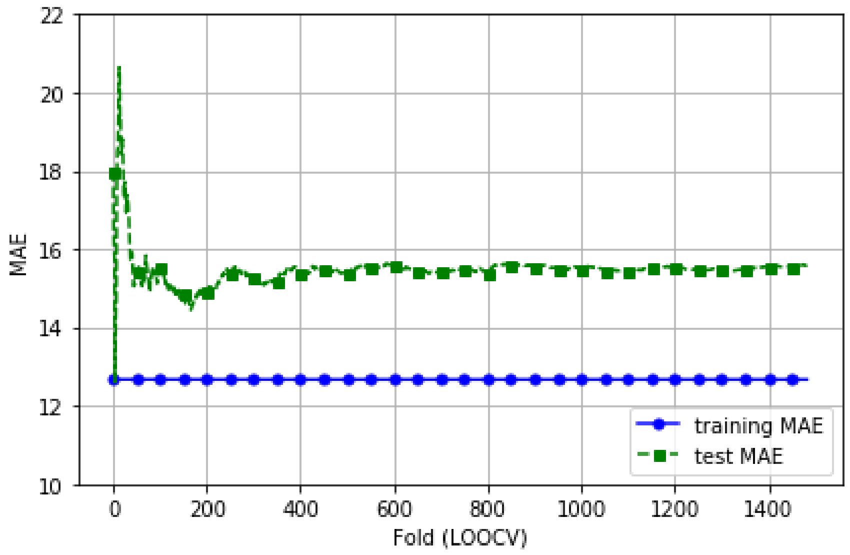
[15]:
```
metrics_loocv, means_loocv, std_loocv = loocv(X, y, n_neighbors)
```

```
148 / 1483 test MSE: 196.0000 std: 331.6123 | train MSE: 233.8279 std: 0.3839
296 / 1483 test MSE: 25.0000 std: 331.4839 | train MSE: 233.0803 std: 0.3811
444 / 1483 test MSE: 64.0000 std: 354.2768 | train MSE: 232.3320 std: 0.3912
592 / 1483 test MSE: 529.0000 std: 365.5174 | train MSE: 233.2213 std: 0.4085
740 / 1483 test MSE: 324.0000 std: 365.7593 | train MSE: 233.5850 std: 0.4091
888 / 1483 test MSE: 16.0000 std: 386.1413 | train MSE: 233.6242 std: 0.4082
1036 / 1483 test MSE: 169.0000 std: 392.5298 | train MSE: 233.2429 std: 0.4095
1184 / 1483 test MSE: 784.0000 std: 399.4872 | train MSE: 233.8327 std: 0.4143
1332 / 1483 test MSE: 324.0000 std: 391.1226 | train MSE: 233.6316 std: 0.4085
1480 / 1483 test MSE: 81.0000 std: 401.0179 | train MSE: 233.8792 std: 0.4104
Done!
```

[16]:
```
train_mean = means_loocv[:,2]
train_std = std_loocv[:,2]
test_mean = means_loocv[:,0]
test_std = std_loocv[:,0]

n = X.shape[0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=n,
                markevery=50,
                xlab='Fold (LOOCV)',
                ylab='MSE',
                lim=[150, 500],
                file='MSE_holdoutLOOCV',
                std=False)
```



[17]:
```
train_mean = means_loocv[:,3]
train_std = std_loocv[:,3]
test_mean = means_loocv[:,1]
test_std = std_loocv[:,1]

n = X.shape[0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=n,
                markevery=50,
                xlab='Fold (LOOCV)',
                ylab='MAE',
                lim=[10, 22],
                file='MAE_holdoutLOOCV',
                std=False)
```



1.4 10-fold Cross-Validation (CV)

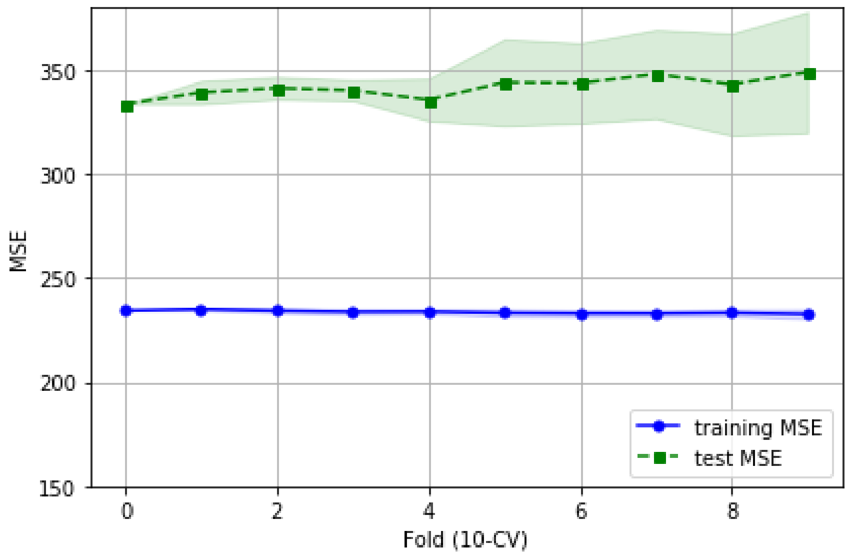
```
[18]: def k_fold_cv(X, y, n_neighbors, folds, seed=1, log=True):

          n = folds

          metrics, means, std = [np.empty((folds,4)) for _ in range(3)]

          cv = KFold(n_splits=folds, shuffle=True, random_state=seed)

          for index, (train_index, test_index) in enumerate(cv.split(X, y)):

              V = np.cov(X[train_index].T)

              KNN_regressor = KNeighborsRegressor(n_neighbors=n_neighbors,
                                                  weights='uniform',
                                                  algorithm='auto',
                                                  metric='mahalanobis',
                                                  metric_params={'V':V})

              KNN_regressor.fit(X[train_index], y[train_index])
```

```
        pred_test = KNN_regressor.predict(X[test_index])
        pred_train = KNN_regressor.predict(X[train_index])
        metrics[index,:] = MSE(y[test_index], pred_test), MAE(y[test_index],␣
↪pred_test), MSE(y[train_index], pred_train), MAE(y[train_index], pred_train)
        means[index,:] = np.mean(metrics[:(index+1)], axis=0)
        std[index,:] = np.std(metrics[:(index+1)], axis=0)

        if ((index+1) % (int(n/10)) == 0) & log:
            print(f"{index+1} / {n} test MSE: {metrics[index,:][0]:.4f} std:␣
↪{std[index,:][0]:.4f} | train MSE: {metrics[index,:][2]:.4f} std:␣
↪{std[index,:][2]:.4f}")
    if log:
        print("Done!")

    return metrics, means, std
```

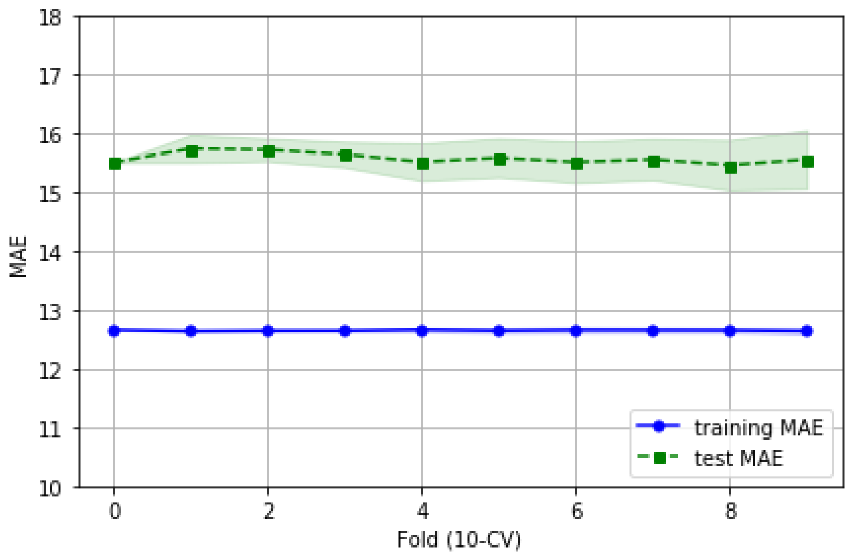
[19]:
```
folds = 10

metrics_cv, means_cv, std_cv = k_fold_cv(X, y, n_neighbors, folds)
```

```
1 / 10 test MSE: 333.8188 std: 0.0000 | train MSE: 234.4640 std: 0.0000
2 / 10 test MSE: 345.0268 std: 5.6040 | train MSE: 235.7346 std: 0.6353
3 / 10 test MSE: 345.6242 std: 5.4298 | train MSE: 232.9655 std: 1.1318
4 / 10 test MSE: 337.3784 std: 5.0281 | train MSE: 232.3805 std: 1.3101
5 / 10 test MSE: 317.7027 std: 10.1540 | train MSE: 234.2989 std: 1.1833
6 / 10 test MSE: 385.8041 std: 20.7767 | train MSE: 230.2442 std: 1.7589
7 / 10 test MSE: 341.6959 std: 19.2558 | train MSE: 231.8524 std: 1.7104
8 / 10 test MSE: 378.5878 std: 21.3615 | train MSE: 232.9011 std: 1.6018
9 / 10 test MSE: 303.5541 std: 24.5463 | train MSE: 235.4629 std: 1.6822
10 / 10 test MSE: 401.5473 std: 29.1240 | train MSE: 227.3431 std: 2.4110
Done!
```

[20]:
```
train_mean = means_cv[:,2]
train_std = std_cv[:,2]
test_mean = means_cv[:,0]
test_std = std_cv[:,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=folds,
                markevery=1,
                xlab='Fold (10-CV)',
                ylab='MSE',
                lim=[150, 380],
                file='MSE_holdout10Fold')
```



```
[21]: train_mean = means_cv[:,3]
      train_std = std_cv[:,3]
      test_mean = means_cv[:,1]
      test_std = std_cv[:,1]

      plot_train_test(train_mean,
                      train_std,
                      test_mean,
                      test_std,
                      length=folds,
                      markevery=1,
                      xlab='Fold (10-CV)',
                      ylab='MAE',
                      lim=[10, 18],
                      file='MAE_holdout10Fold')
```



1.5 Nested 10-fold Cross Validation (N-10-CV)

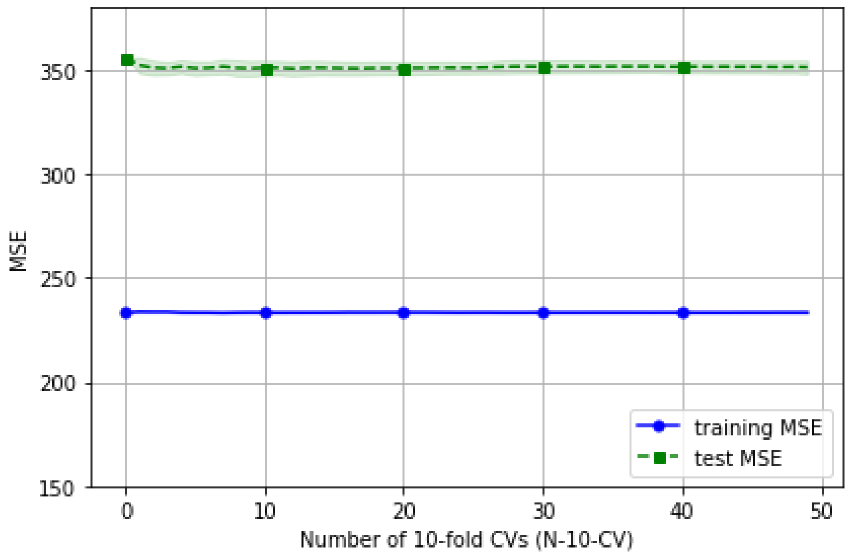
[24]:
```
def nested_k_fold_cv(X, y, n_neighbors, folds, n, log=True, seed=12345):

    rng = np.random.RandomState(seed=seed)
    seeds = np.arange(10**5); rng.shuffle(seeds); seeds=seeds[:n]

    metrics, means, std = [np.empty((n,4)) for _ in range(3)]

    for index in range(n):

        metrics_cv, *_ = k_fold_cv(X, y, n_neighbors, folds, seed=seeds[index],␣
↪log=False)

        metrics[index,:] = np.mean(metrics_cv, axis=0)
        means[index,:] = np.mean(metrics[:(index+1)], axis=0)
        std[index,:] = np.std(metrics[:(index+1)], axis=0)

        if ((index+1) % (int(n/10)) == 0) & log:
            print(f"{index+1} / {n} test MSE: {metrics[index,:][0]:.4f} std:␣
↪{std[index,:][0]:.4f} | train MSE: {metrics[index,:][2]:.4f} std:␣
↪{std[index,:][2]:.4f}")
```

```
    if log:
        print("Done!")

    return metrics, means, std
```

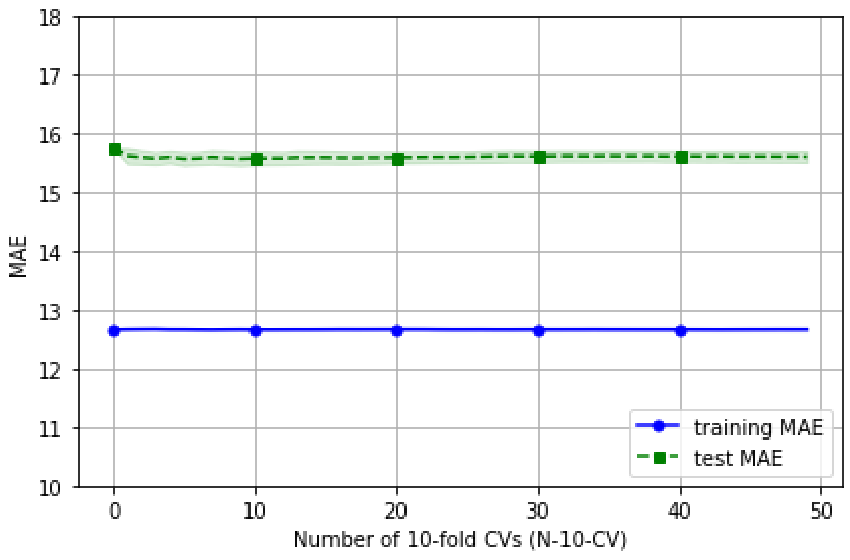
[25]:
```
n = 50
folds = 10

metrics_ncv, means_ncv, std_ncv = nested_k_fold_cv(X, y, n_neighbors, folds, n)
```

```
5 / 50 test MSE: 355.0425 std: 3.2412 | train MSE: 232.6091 std: 0.5724
10 / 50 test MSE: 349.0768 std: 3.7088 | train MSE: 234.3002 std: 0.5986
15 / 50 test MSE: 352.0713 std: 3.4905 | train MSE: 233.8118 std: 0.5324
20 / 50 test MSE: 350.7849 std: 3.1969 | train MSE: 234.0268 std: 0.5514
25 / 50 test MSE: 350.3358 std: 2.9295 | train MSE: 232.9113 std: 0.5916
30 / 50 test MSE: 352.1791 std: 3.2342 | train MSE: 234.1941 std: 0.5851
35 / 50 test MSE: 350.0629 std: 3.0778 | train MSE: 234.2456 std: 0.5582
40 / 50 test MSE: 346.0720 std: 3.0500 | train MSE: 234.0835 std: 0.5413
45 / 50 test MSE: 347.9022 std: 3.0950 | train MSE: 234.8433 std: 0.5577
50 / 50 test MSE: 343.9117 std: 3.2539 | train MSE: 233.9725 std: 0.5686
Done!
```

[26]:
```
train_mean = means_ncv[:,2]
train_std = std_ncv[:,2]
test_mean = means_ncv[:,0]
test_std = std_ncv[:,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=n,
                markevery=10,
                xlab='Number of 10-fold CVs (N-10-CV)',
                ylab='MSE',
                lim=[150, 380],
                file='MSE_N-10-CV')
```



[27]:
```
train_mean = means_ncv[:,3]
train_std = std_ncv[:,3]
test_mean = means_ncv[:,1]
test_std = std_ncv[:,1]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=n,
                markevery=10,
                xlab='Number of 10-fold CVs (N-10-CV)',
                ylab='MAE',
                lim=[10, 18],
                file='MAE_N-10-CV')
```



1.6 Bootstrapping

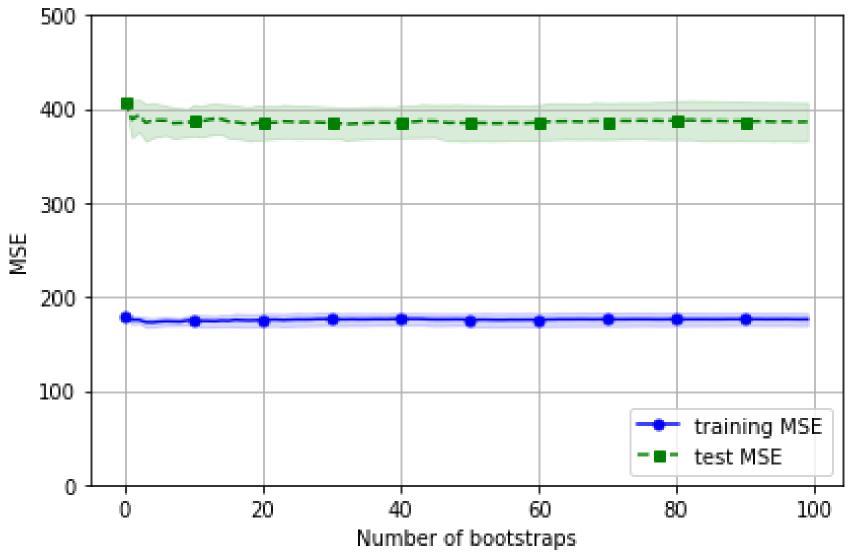
[51]:
```python
def bootstrap(X, y, bootstraps, n_neighbors, test_size, seed=12345, log=True):

    rng = np.random.RandomState(seed=seed)

    X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                        test_size=test_size,
                                                        random_state=seed)

    metrics, means, std = [np.empty((bootstraps,4)) for _ in range(3)]

    sample_size = X_train.shape[0]

    for index in range(bootstraps):

        bootstrap = np.random.choice(np.arange(sample_size), sample_size,␣
↪replace=True)
        X_bootstrap = X_train[bootstrap]
        y_bootstrap = y_train[bootstrap]

        V = np.cov(X_bootstrap.T)
        KNN_regressor = KNeighborsRegressor(n_neighbors=n_neighbors,
                                             weights='uniform',
                                             algorithm='auto',
                                             metric='mahalanobis',
                                             metric_params={'V':V})

        KNN_regressor.fit(X_bootstrap, y_bootstrap)
        pred_test = KNN_regressor.predict(X_test)
        pred_train = KNN_regressor.predict(X_bootstrap)
        metrics[index,:] = MSE(y_test, pred_test), MAE(y_test, pred_test),␣
 ↪MSE(y_bootstrap, pred_train), MAE(y_bootstrap, pred_train)
        means[index,:] = np.mean(metrics[:(index+1)], axis=0)
        std[index,:] = np.std(metrics[:(index+1)], axis=0)

        if ((index+1) % (int(bootstraps/10)) == 0) & log:
            print(f"{index+1} / {bootstraps} test MSE: {metrics[index,:][0]:.
 ↪4f} std: {std[index,:][0]:.4f} | train MSE: {metrics[index,:][2]:.4f} std:␣
 ↪{std[index,:][2]:.4f}")

    if log:
        print("Done!")

    return metrics, means, std
```

[31]:
```
bootstraps=100

metrics_bt, means_bt, std_bt = bootstrap(X, y, bootstraps,␣
 ↪n_neighbors=n_neighbors, seed=1, test_size=test_size)
```

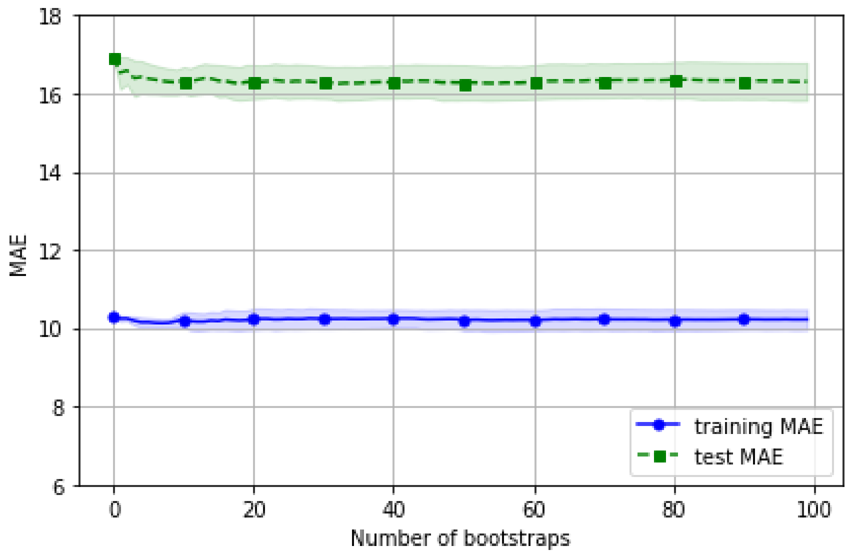
```
10 / 100 test MSE: 384.7778 std: 14.7781 | train MSE: 185.3238 std: 5.3455
20 / 100 test MSE: 412.8283 std: 18.5174 | train MSE: 179.0708 std: 6.8588
30 / 100 test MSE: 377.7710 std: 16.8659 | train MSE: 177.5455 std: 6.9913
40 / 100 test MSE: 377.8653 std: 16.3323 | train MSE: 185.3221 std: 6.6029
50 / 100 test MSE: 357.9461 std: 19.5534 | train MSE: 172.6071 std: 6.5762
60 / 100 test MSE: 411.4916 std: 18.7154 | train MSE: 176.0599 std: 7.3774
70 / 100 test MSE: 372.0875 std: 19.7512 | train MSE: 183.2926 std: 7.3267
80 / 100 test MSE: 416.9630 std: 20.2306 | train MSE: 184.8870 std: 7.1485
90 / 100 test MSE: 394.0202 std: 20.8136 | train MSE: 177.0911 std: 6.9658
100 / 100 test MSE: 400.3771 std: 20.5983 | train MSE: 178.9030 std: 6.9311
Done!
```

[143]:
```
train_mean = means_bt[:,2]
train_std = std_bt[:,2]
test_mean = means_bt[:,0]
test_std = std_bt[:,0]
```

```
plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=bootstraps,
                markevery=10,
                xlab='Number of bootstraps',
                ylab='MSE',
                lim=[0, 500],
                file='MSE_bootstraps100')
```



[34]:
```
train_mean = means_bt[:,3]
train_std = std_bt[:,3]
test_mean = means_bt[:,1]
test_std = std_bt[:,1]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=bootstraps,
                markevery=10,
                xlab='Number of bootstraps',
                ylab='MAE',
                lim=[6, 18],
                file='MAE_bootstraps100')
```



2 Question 3 - varying K

[22]:
```
max_k = 20
parameters = range(1,max_k+1)
```

2.1 Holdout

[23]:
```
metrics_hld = np.empty((max_k,4))

rng = np.random.RandomState(seed=12345)
seeds = np.arange(10**5); rng.shuffle(seeds); seeds=seeds[:max_k+1]

for parameter in parameters:

    X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                        test_size=test_size,
                                                                    ␣
↪random_state=seeds[parameter])
   V = np.cov(X_train.T)

   KNN_regressor = KNeighborsRegressor(n_neighbors=parameter,
                                       weights='uniform',
                                       algorithm='auto',
                                       metric='mahalanobis',
                                       metric_params={'V':V})

   KNN_regressor.fit(X_train, y_train)
   pred_train = KNN_regressor.predict(X_train)
   pred_test = KNN_regressor.predict(X_test)

   metrics_hld[parameter-1,] = MSE(y_test, pred_test), MAE(y_test, pred_test),␣
↪MSE(y_train, pred_train), MAE(y_train, pred_train)
```

2.2 Repeated holdout

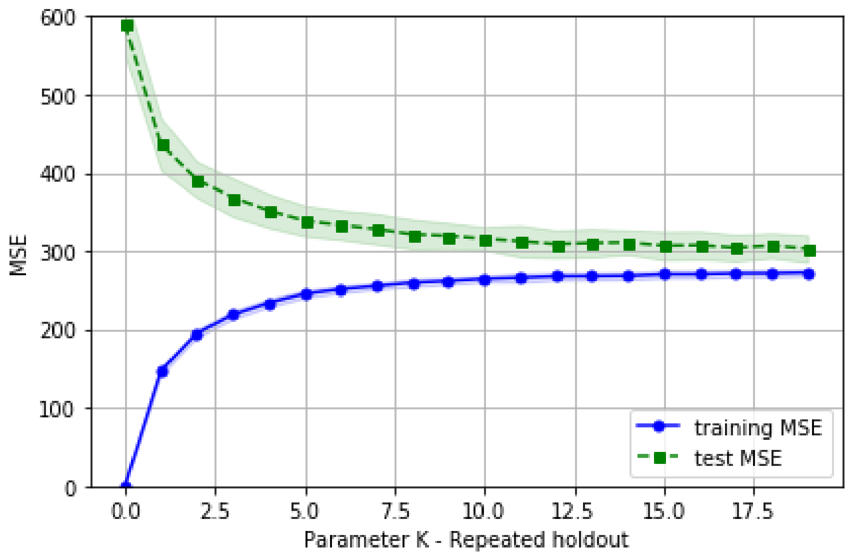
```
[67]: def iterate_over_param(X, y, max_k, evaluation_model, model_param,␣
↪parameter_key, seeds_required=True, seed=12345):

   means_param, std_param = [np.empty((max_k,4)) for _ in range(2)]

   rng = np.random.RandomState(seed=seed)
   seeds = np.arange(10**5); rng.shuffle(seeds); seeds=seeds[:max_k+1]

   parameters = range(1,max_k+1)

   for parameter in parameters:

       if seeds_required:
           model_param['seed'] = seeds[parameter]

       model_param[parameter_key] = parameter

       metrics, means, std = evaluation_model(X, y, **model_param)

       means_param[parameter-1,:] = np.mean(metrics, axis=0)
       std_param[parameter-1,:] = np.std(metrics, axis=0)

       print(f"K: {parameter} test MSE: {means_param[parameter-1,:][0]:.4f}␣
↪std: {std_param[parameter-1,:][0]:.4f} | train MSE {means_param[parameter-1,:
↪][2]:.4f} std: {std_param[parameter-1,:][2]:.4f}  ")
```

```
    print("Done")
    return means_param, std_param
```

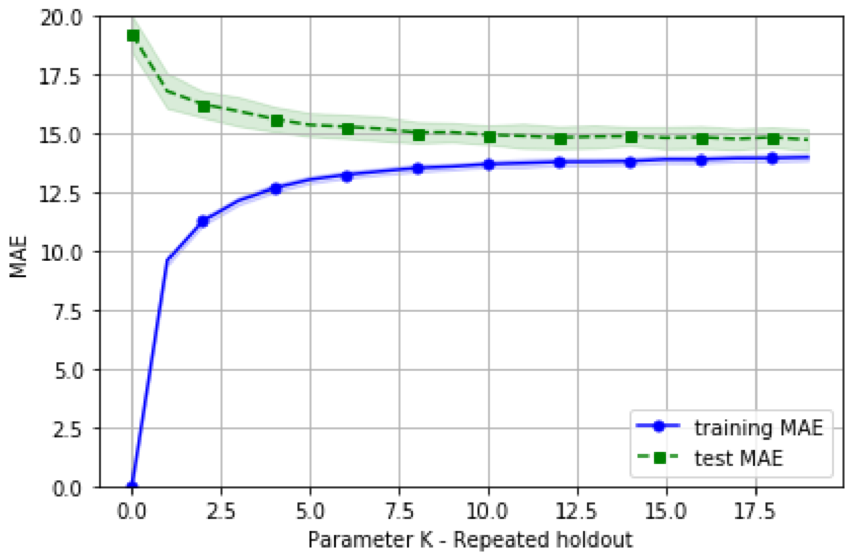
[68]:
```
n = 100

means_rph, std_rph = iterate_over_param(X, y, max_k, repeated_holdout, {'n':n,␣
↪'test_size':test_size, 'log':False}, parameter_key='n_neighbors')
```

```
K: 1 test MSE: 589.8867 std: 39.6774 | train MSE 0.0000 std: 0.0000
K: 2 test MSE: 436.5609 std: 33.3337 | train MSE 147.0484 std: 4.6982
K: 3 test MSE: 391.3697 std: 23.2022 | train MSE 194.8638 std: 5.1343
K: 4 test MSE: 368.4727 std: 24.6736 | train MSE 218.7596 std: 5.5339
K: 5 test MSE: 351.4719 std: 21.5159 | train MSE 233.9926 std: 5.3611
K: 6 test MSE: 338.7185 std: 19.4866 | train MSE 245.3678 std: 5.0929
K: 7 test MSE: 333.1704 std: 18.6027 | train MSE 251.4303 std: 4.8013
K: 8 test MSE: 328.1909 std: 19.5116 | train MSE 255.4400 std: 4.5051
K: 9 test MSE: 321.5185 std: 18.8735 | train MSE 259.7628 std: 5.2588
K: 10 test MSE: 319.6372 std: 16.4494 | train MSE 261.8980 std: 4.4692
K: 11 test MSE: 315.9609 std: 14.9359 | train MSE 264.6539 std: 4.2197
K: 12 test MSE: 312.6581 std: 20.2725 | train MSE 266.1061 std: 5.8329
K: 13 test MSE: 308.9278 std: 17.7489 | train MSE 267.8839 std: 5.2129
K: 14 test MSE: 310.3434 std: 18.1785 | train MSE 268.1025 std: 4.9196
K: 15 test MSE: 311.0403 std: 15.6909 | train MSE 268.4938 std: 4.8013
K: 16 test MSE: 306.8919 std: 18.1993 | train MSE 270.4770 std: 5.2744
K: 17 test MSE: 307.5071 std: 18.0296 | train MSE 270.5379 std: 5.2281
K: 18 test MSE: 304.2399 std: 16.9018 | train MSE 271.7011 std: 4.5681
K: 19 test MSE: 307.0235 std: 16.1057 | train MSE 271.7121 std: 4.9070
K: 20 test MSE: 303.1302 std: 17.1427 | train MSE 272.7445 std: 4.7932
Done
```

[69]:
```
train_mean = means_rph[:,2]
train_std = std_rph[:,2]
test_mean = means_rph[:,0]
test_std = std_rph[:,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=max_k,
                markevery=1,
                xlab='Parameter K - Repeated holdout',
                ylab='MSE',
                lim=[0, 600],
                file='MSE_RepeatedHoldoutKOptimize')
```



```
[81]: train_mean = means_rph[:,3]
      train_std = std_rph[:,3]
      test_mean = means_rph[:,1]
      test_std = std_rph[:,1]

      plot_train_test(train_mean,
                      train_std,
                      test_mean,
                      test_std,
                      length=max_k,
                      markevery=2,
                      xlab='Parameter K - Repeated holdout',
                      ylab='MAE',
                      lim=[0, 20],
                      file='MAE_RepeatedHoldoutKOptimize')
```



2.3 Leave-One-Out Cross-Validation (LOOCV)

[38]:
```
#Let op, dit ding is pas klaar tegen de tijd dat je 80 bent
means_loocv_po, std_loocv_po = iterate_over_param(X, y, max_k, loocv, {'log':
 ↪False}, parameter_key='n_neighbors')
```

```
K: 1 test MSE: 582.5239 std: 748.1722 | train MSE 0.0000 std: 0.0000
K: 2 test MSE: 443.0283 std: 568.7768 | train MSE 145.7477 std: 0.2892
K: 3 test MSE: 388.5664 std: 474.9134 | train MSE 197.3279 std: 0.4153
K: 4 test MSE: 364.8409 std: 431.2678 | train MSE 218.7633 std: 0.5172
K: 5 test MSE: 349.0405 std: 402.8348 | train MSE 233.6128 std: 0.4128
K: 6 test MSE: 343.8874 std: 395.4071 | train MSE 242.6467 std: 0.3761
K: 7 test MSE: 334.7067 std: 384.9329 | train MSE 253.1216 std: 0.3865
K: 8 test MSE: 327.3223 std: 372.0058 | train MSE 256.6894 std: 0.3801
K: 9 test MSE: 320.6231 std: 362.0866 | train MSE 259.8104 std: 0.3536
K: 10 test MSE: 320.0688 std: 359.4104 | train MSE 260.0634 std: 0.3677
K: 11 test MSE: 318.1955 std: 358.8949 | train MSE 263.7839 std: 0.3439
K: 12 test MSE: 317.1382 std: 356.9212 | train MSE 268.0253 std: 0.3564
K: 13 test MSE: 313.0701 std: 349.8855 | train MSE 270.6852 std: 0.3702
K: 14 test MSE: 309.5752 std: 345.6595 | train MSE 269.9048 std: 0.3301
K: 15 test MSE: 308.2960 std: 342.7709 | train MSE 269.5563 std: 0.3541
K: 16 test MSE: 306.9063 std: 340.8787 | train MSE 271.1552 std: 0.3279
```

```
K: 17 test MSE: 305.4734 std: 337.0741 | train MSE 272.3143 std: 0.3182
K: 18 test MSE: 304.9582 std: 335.7122 | train MSE 272.8552 std: 0.3453
K: 19 test MSE: 304.0115 std: 334.5281 | train MSE 273.3501 std: 0.3188
K: 20 test MSE: 302.1827 std: 331.4328 | train MSE 273.8528 std: 0.3139
Done
```

[ ]:
```
train_mean = means_loocv_po[:,2]
train_std = std_loocv_po[:,2]
test_mean = means_loocv_po[:,0]
test_std = std_loocv_po[:,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=max_k,
                markevery=1,
                xlab='Parameter K - LOOCV',
                ylab='MSE',
                lim=[150, 380],
                file='MSE_LOOCVKOptimize',
                std=False)
```

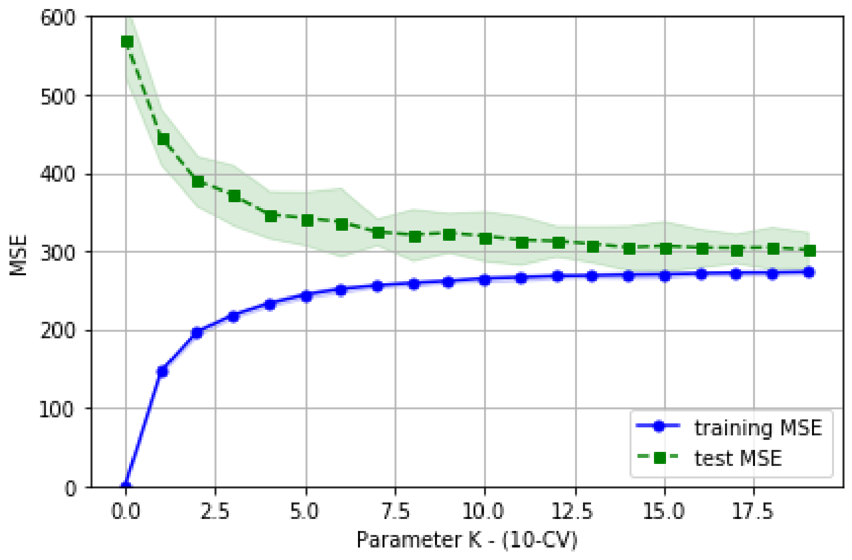
[ ]:
```
train_mean = means_loocv_po[:,3]
train_std = std_loocv_po[:,3]
test_mean = means_loocv_po[:,1]
test_std = std_loocv_po[:,1]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=max_k,
                markevery=2,
                xlab='Parameter K -LOOCV',
                ylab='MAE',
                lim=[0, 20],
                file='MAE_LOOCVKOptimize',
                std=False)
```

2.4 10-fold Cross-Validation (CV)

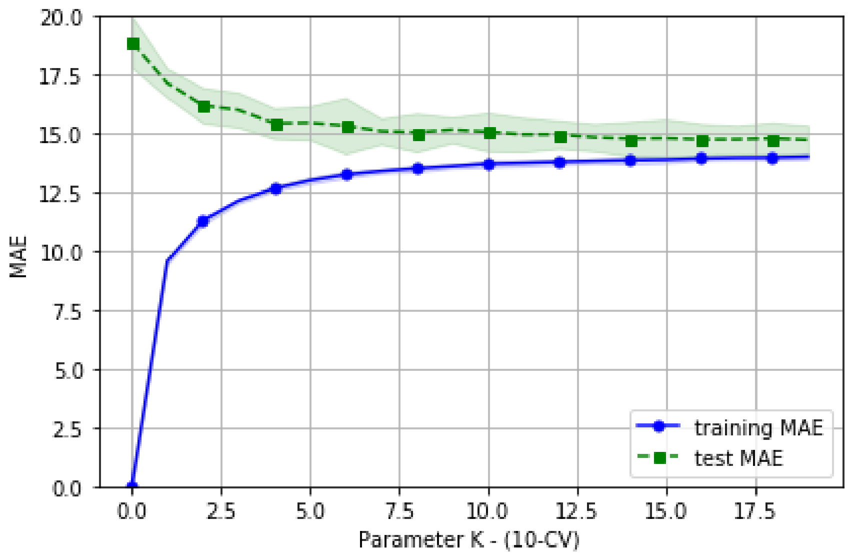
[71]:
```
folds = 10

means_10cv_po, std_10cv_po = iterate_over_param(X, y, max_k, k_fold_cv,␣
 ↪{'folds':folds, 'log':False}, parameter_key='n_neighbors')
```

```
K: 1 test MSE: 571.1905 std: 48.2308 | train MSE 0.0000 std: 0.0000
K: 2 test MSE: 445.9161 std: 35.3493 | train MSE 146.3110 std: 2.8454
K: 3 test MSE: 389.8379 std: 32.1153 | train MSE 196.4947 std: 4.4452
K: 4 test MSE: 371.9971 std: 38.4374 | train MSE 218.1978 std: 3.4077
K: 5 test MSE: 346.9770 std: 29.9678 | train MSE 233.3586 std: 4.0619
K: 6 test MSE: 342.1246 std: 34.0909 | train MSE 244.1285 std: 3.6210
K: 7 test MSE: 337.2262 std: 43.5189 | train MSE 251.4821 std: 4.5765
K: 8 test MSE: 324.9382 std: 16.8347 | train MSE 256.0207 std: 2.2092
K: 9 test MSE: 321.1391 std: 32.8618 | train MSE 259.1189 std: 4.0215
K: 10 test MSE: 323.5690 std: 25.3226 | train MSE 261.8165 std: 2.3706
K: 11 test MSE: 319.4833 std: 31.6956 | train MSE 265.0826 std: 3.9311
K: 12 test MSE: 314.4074 std: 30.7413 | train MSE 266.5610 std: 4.3910
K: 13 test MSE: 312.9323 std: 19.7058 | train MSE 268.2459 std: 3.2658
K: 14 test MSE: 309.3248 std: 23.0097 | train MSE 268.9822 std: 3.0545
K: 15 test MSE: 304.7782 std: 28.1240 | train MSE 269.8466 std: 4.5405
K: 16 test MSE: 306.6561 std: 31.6770 | train MSE 270.3232 std: 4.4088
K: 17 test MSE: 304.5431 std: 24.2582 | train MSE 271.7366 std: 2.4115
K: 18 test MSE: 304.1122 std: 18.7014 | train MSE 272.5126 std: 2.8394
K: 19 test MSE: 304.6998 std: 26.6535 | train MSE 272.6829 std: 2.8604
K: 20 test MSE: 301.6786 std: 23.2309 | train MSE 273.5396 std: 2.9509
Done
```

[80]:
```
train_mean = means_10cv_po[:,2]
train_std = std_10cv_po[:,2]
test_mean = means_10cv_po[:,0]
test_std = std_10cv_po[:,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=max_k,
                markevery=1,
                xlab='Parameter K - (10-CV)',
                ylab='MSE',
                lim=[0, 600],
                file='MSE_10CVKOptimize')
```



[73]:
```
train_mean = means_10cv_po[:,3]
train_std = std_10cv_po[:,3]
test_mean = means_10cv_po[:,1]
test_std = std_10cv_po[:,1]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=max_k,
                markevery=2,
                xlab='Parameter K - (10-CV)',
                ylab='MAE',
                lim=[0, 20],
                file='MAE_10CVKOptimize')
```



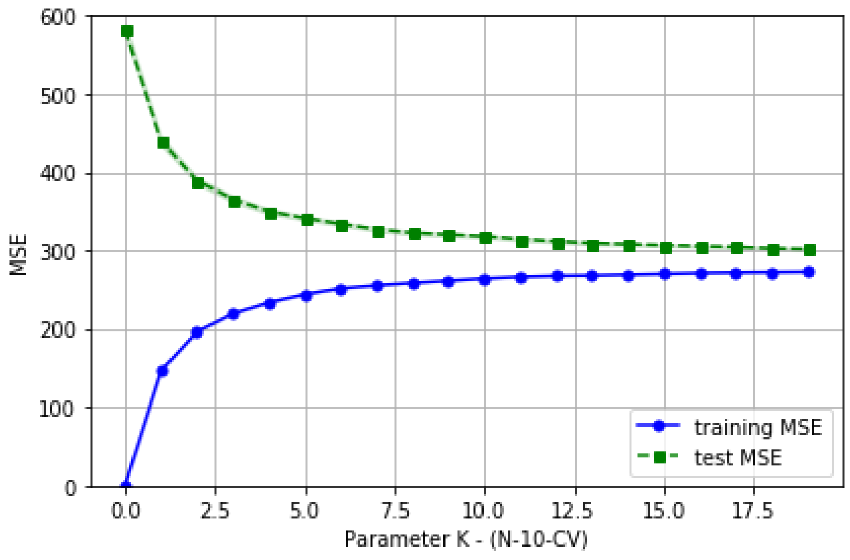
2.5 Nested 10-fold Cross Validation (N-10-CV)

```
[ ]: folds = 10
     n = 50

     means_n10cv_po, std_n10cv_po = iterate_over_param(X, y, max_k,␣
      ↪nested_k_fold_cv, {'folds':folds, 'log':False, 'n':n},␣
      ↪parameter_key='n_neighbors')
```

```
K: 1 test MSE: 582.2137 std: 8.9164 | train MSE 0.0000 std: 0.0000
K: 2 test MSE: 440.4750 std: 6.0598 | train MSE 146.4388 std: 0.3520
K: 3 test MSE: 389.3825 std: 4.6085 | train MSE 196.0401 std: 0.5851
K: 4 test MSE: 365.9229 std: 4.0198 | train MSE 219.2758 std: 0.4384
K: 5 test MSE: 350.1589 std: 3.4860 | train MSE 233.6098 std: 0.4451
K: 6 test MSE: 341.4170 std: 2.7376 | train MSE 244.1132 std: 0.5045
K: 7 test MSE: 334.0701 std: 2.5590 | train MSE 251.7987 std: 0.4639
K: 8 test MSE: 327.2632 std: 2.5801 | train MSE 255.7547 std: 0.4200
K: 9 test MSE: 322.6320 std: 2.6188 | train MSE 258.9929 std: 0.3787
K: 10 test MSE: 320.3858 std: 2.3470 | train MSE 261.8078 std: 0.3271
K: 11 test MSE: 317.9918 std: 2.1765 | train MSE 264.7149 std: 0.4091
K: 12 test MSE: 314.3987 std: 2.5388 | train MSE 266.8235 std: 0.3366
K: 13 test MSE: 311.5021 std: 1.9367 | train MSE 268.1440 std: 0.3379
```

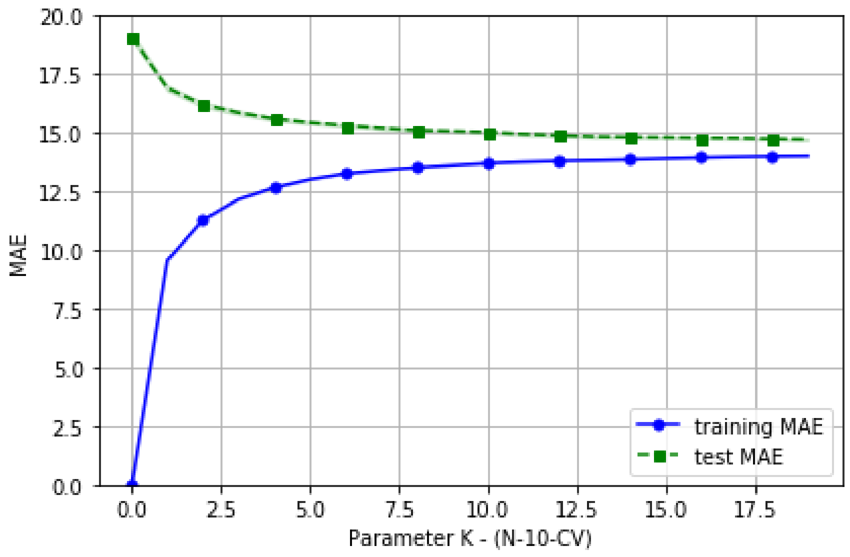
```
K: 14 test MSE: 309.1281 std: 2.2864 | train MSE 268.6703 std: 0.2656
K: 15 test MSE: 307.7209 std: 1.5121 | train MSE 269.6205 std: 0.2679
K: 16 test MSE: 306.5121 std: 1.4399 | train MSE 270.7130 std: 0.2482
K: 17 test MSE: 305.2683 std: 1.7066 | train MSE 271.7133 std: 0.2621
```

[7]:
```
train_mean = means_n10cv_po[:,2]
train_std = std_n10cv_po[:,2]
test_mean = means_n10cv_po[:,0]
test_std = std_n10cv_po[:,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=max_k,
                markevery=1,
                xlab='Parameter K - (N-10-CV)',
                ylab='MSE',
                lim=[0, 600],
                file='MSE_N10CVKOptimize')
```



[8]:
```
train_mean = means_n10cv_po[:,3]
train_std = std_n10cv_po[:,3]
test_mean = means_n10cv_po[:,1]
```

```
test_std = std_n10cv_po[:,1]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=max_k,
                markevery=2,
                xlab='Parameter K - (N-10-CV)',
                ylab='MAE',
                lim=[0, 20],
                file='MAE_N10CVKOptimize')
```

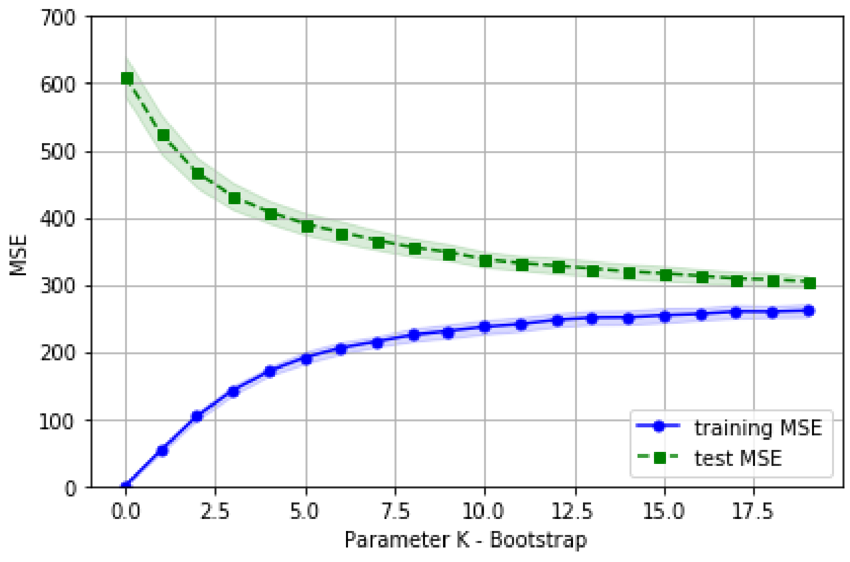


2.6 Bootstrapping

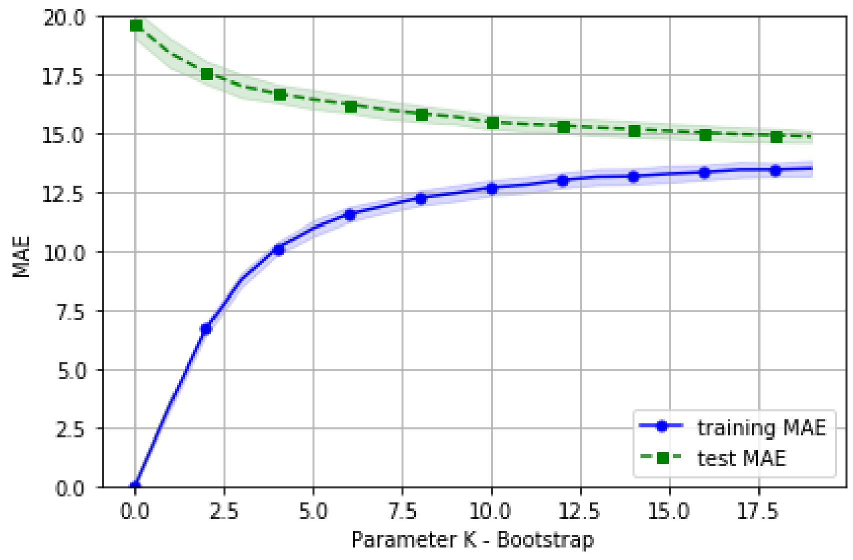
[77]:
```
bootstraps = 100

means_bt_po, std_bt_po = iterate_over_param(X,
                                            y,
                                            max_k, bootstrap,
                                            {'bootstraps':bootstraps,␣
 ↪'test_size':test_size, 'log':False},
                                            parameter_key='n_neighbors',
                                            seeds_required=False)
```

```
K: 1 test MSE: 611.1443 std: 29.9000 | train MSE 0.0000 std: 0.0000
K: 2 test MSE: 524.6228 std: 28.8484 | train MSE 53.3512 std: 3.9677
K: 3 test MSE: 467.2955 std: 22.5694 | train MSE 104.1217 std: 5.7555
K: 4 test MSE: 431.7866 std: 19.8023 | train MSE 142.3785 std: 7.1757
K: 5 test MSE: 408.6459 std: 16.8738 | train MSE 170.9169 std: 6.5186
K: 6 test MSE: 390.8214 std: 16.1356 | train MSE 191.2731 std: 8.9465
K: 7 test MSE: 378.5712 std: 15.9205 | train MSE 205.8030 std: 8.9614
K: 8 test MSE: 366.4157 std: 14.5744 | train MSE 215.5136 std: 7.8168
K: 9 test MSE: 355.6432 std: 13.6275 | train MSE 225.2856 std: 9.4096
K: 10 test MSE: 348.4401 std: 12.0371 | train MSE 230.8056 std: 10.0156
K: 11 test MSE: 337.7030 std: 11.4399 | train MSE 236.8911 std: 10.1917
K: 12 test MSE: 332.2981 std: 10.5246 | train MSE 241.0690 std: 10.4308
K: 13 test MSE: 328.5549 std: 11.8696 | train MSE 247.3623 std: 10.2362
K: 14 test MSE: 324.2676 std: 11.2580 | train MSE 250.8508 std: 10.4869
K: 15 test MSE: 319.8751 std: 11.2043 | train MSE 251.2633 std: 10.4478
K: 16 test MSE: 316.9539 std: 11.1452 | train MSE 254.4114 std: 11.2303
K: 17 test MSE: 313.2545 std: 10.4270 | train MSE 256.4146 std: 9.5568
K: 18 test MSE: 309.2250 std: 10.2109 | train MSE 260.1437 std: 10.0819
K: 19 test MSE: 307.6848 std: 10.7229 | train MSE 259.8660 std: 8.7903
K: 20 test MSE: 304.8919 std: 8.3818 | train MSE 261.5500 std: 9.9734
Done
```

[78]:
```
train_mean = means_bt_po[:,2]
train_std = std_bt_po[:,2]
test_mean = means_bt_po[:,0]
test_std = std_bt_po[:,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=max_k,
                markevery=1,
                xlab='Parameter K - Bootstrap',
                ylab='MSE',
                lim=[0, 700],
                file='MSE_Bootstrap100Optimize')
```



```
[79]: train_mean = means_bt_po[:,3]
      train_std = std_bt_po[:,3]
      test_mean = means_bt_po[:,1]
      test_std = std_bt_po[:,1]

      plot_train_test(train_mean,
                      train_std,
                      test_mean,
                      test_std,
                      length=max_k,
                      markevery=2,
                      xlab='Parameter K - Bootstrap',
                      ylab='MAE',
                      lim=[0, 20],
                      file='MAE_Bootstrap100Optimize')
```

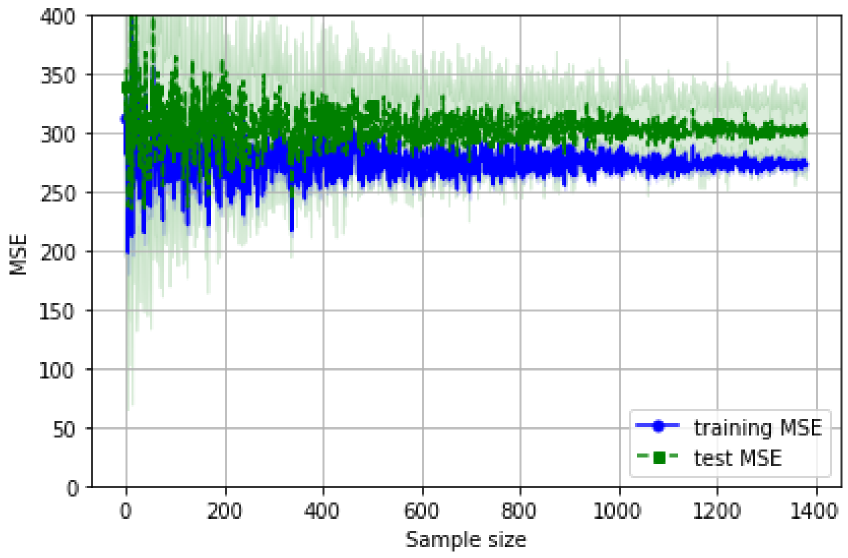


[89]:
```
#Learning curve

sample_size = X.shape[0]
number_of_obs = sample_size-50

means_lc, std_lc = [np.empty((number_of_obs,4)) for _ in range(2)]

for index, size in enumerate(range(50,number_of_obs)):

    sample_index = np.random.choice(np.arange(sample_size), size, replace=False)

    X_lc = X[sample_index]
    y_lc = y[sample_index]

    metrics_cvl, means_cvl, std_cvl = k_fold_cv(X_lc, y_lc, 20, 10, log=False)

    means_lc[index,:] = np.mean(metrics_cvl, axis=0)
    std_lc[index,:] = np.std(metrics_cvl, axis=0)
    if ((index+1) % (int(number_of_obs/10)) == 0):
            print(f"{index+1} / {number_of_obs}")

print("Done!")
```

```
143 / 1433
```

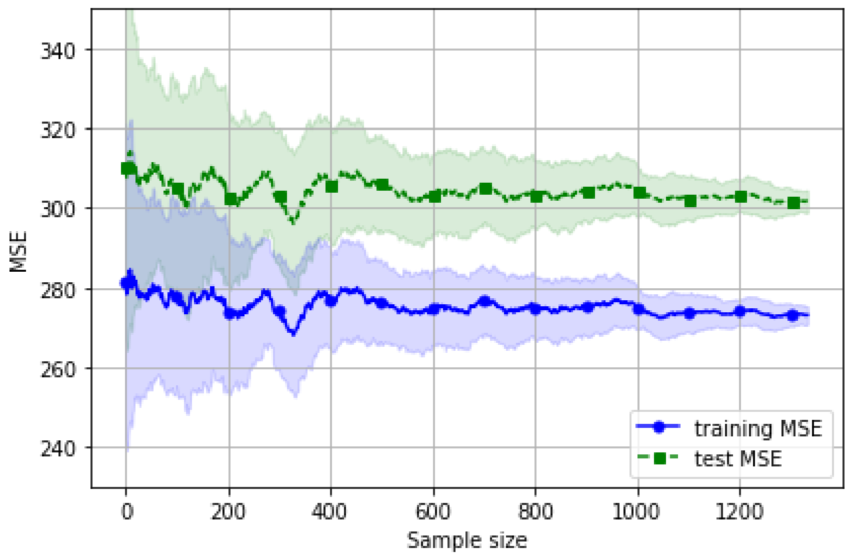
```
286 / 1433
429 / 1433
572 / 1433
715 / 1433
858 / 1433
1001 / 1433
1144 / 1433
1287 / 1433
Done!
```

[97]:
```
train_mean = means_lc[:number_of_obs-50,2]
train_std = std_lc[:number_of_obs-50,2]
test_mean = means_lc[:number_of_obs-50,0]
test_std = std_lc[:number_of_obs-50,0]

plot_train_test(train_mean,
                train_std,
                test_mean,
                test_std,
                length=number_of_obs-50,
                markevery=100,
                xlab='Sample size',
                ylab='MSE',
                lim=[0, 400],
                file='MSE_LC2')
```



```
[134]: #Creating a rolling average, as the original is quite noisy
       mean_lc_r, std_lc_r = [np.empty((means_lc.shape[0]-100,4)) for _ in range(2)]

       for i in range(means_lc.shape[0]-100):
           mean_lc_r[i,:] = np.mean(means_lc[i:(i+50)],axis=0)
           std_lc_r[i,:] = np.std(means_lc[i:(i+50)],axis=0)
```

```
[128]: train_mean = mean_lc_r[:,2]
       train_std = std_lc_r[:,2]
       test_mean = mean_lc_r[:,0]
       test_std = std_lc_r[:,0]

       plot_train_test(train_mean,
                       train_std,
                       test_mean,
                       test_std,
                       length=mean_lc_r.shape[0],
                       markevery=100,
                       xlab='Sample size',
                       ylab='MSE',
                       lim=[230, 350],
                       file='MSE_LCR3')
```

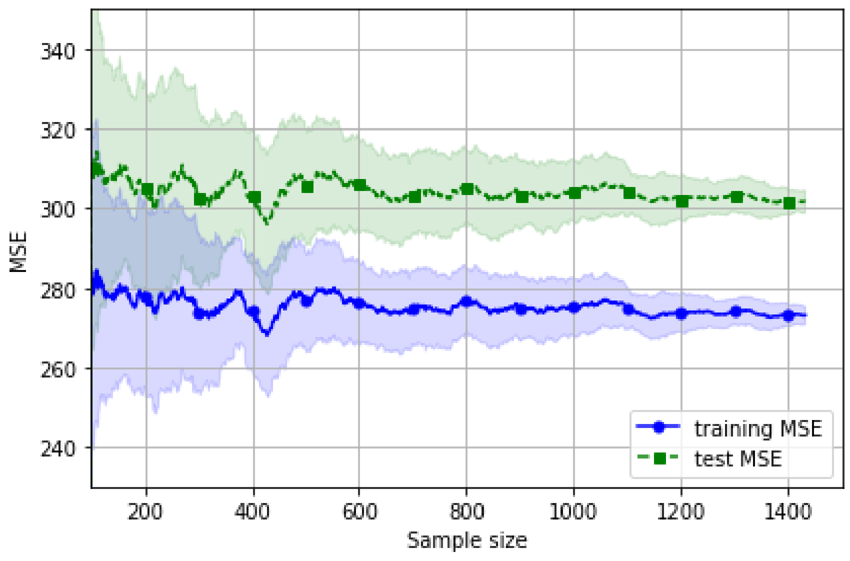


[135]:
```
#This is quite a hacky solution to shift the x-axes of the graph 100 to the␣
↪left.
mean_lc_r_hack = np.zeros((mean_lc_r.shape[0]+100,4))
std_lc_r_hack = np.zeros((mean_lc_r.shape[0]+100,4))

mean_lc_r_hack[100:] = mean_lc_r
std_lc_r_hack[100:] = std_lc_r
```

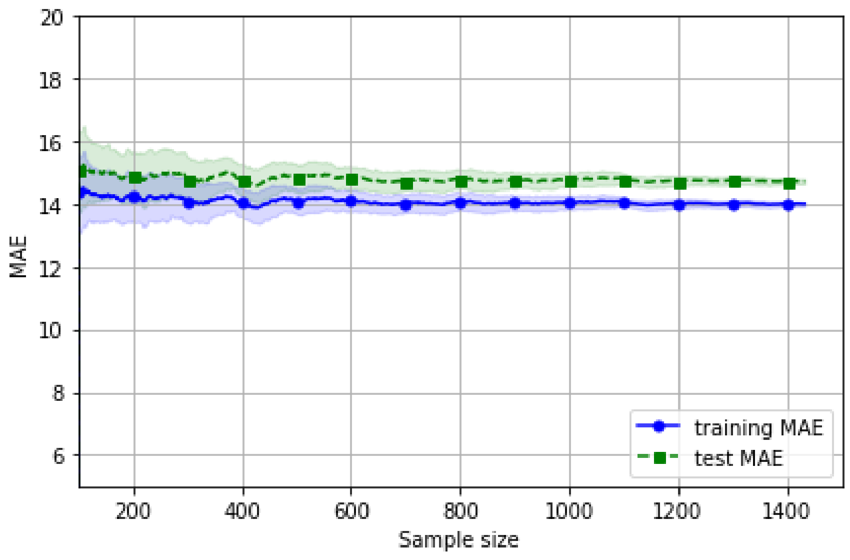
[136]:
```
def plot_train_test_hack(train_mean, train_std, test_mean, test_std, length,␣
↪markevery, xlab, ylab, lim, xlim, file, std=True):

    number_of_repetitions = np.arange(length)

    plt.plot(number_of_repetitions, train_mean,
             color='blue', marker='o',
             markersize=5, label=f'training {ylab}', markevery=markevery)

    plt.plot(number_of_repetitions, test_mean,
             color='green', linestyle='--',
             marker='s', markersize=5,
             label=f'test {ylab}', markevery=markevery)

    if std:
        plt.fill_between(number_of_repetitions,
                         test_mean + test_std,
                         test_mean - test_std,
                         alpha=0.15, color='green')

        plt.fill_between(number_of_repetitions,
                         train_mean + train_std,
                         train_mean - train_std,
                         alpha=0.15, color='blue')

    plt.grid()
    plt.xlabel(f'{xlab}')
    plt.ylabel(f'{ylab}')
    plt.legend(loc='lower right')
    plt.ylim(lim)
    plt.xlim(xlim)
    plt.tight_layout()
    plt.savefig(f'images/{file}.svg', dpi=300)
    plt.show()
```

[142]:
```
train_mean = mean_lc_r_hack[:,2]
train_std = std_lc_r_hack[:,2]
test_mean = mean_lc_r_hack[:,0]
test_std = std_lc_r_hack[:,0]
```

```
plot_train_test_hack(train_mean,
                train_std,
                test_mean,
                test_std,
                length=mean_lc_r_hack.shape[0],
                markevery=100,
                xlab='Sample size',
                ylab='MSE',
                lim=[230, 350],
                xlim=[100,1500],
                file='MSE_LCR4')
```



[146]:
```
train_mean = mean_lc_r_hack[:,3]
train_std = std_lc_r_hack[:,3]
test_mean = mean_lc_r_hack[:,1]
test_std = std_lc_r_hack[:,1]

plot_train_test_hack(train_mean,
                train_std,
                test_mean,
                test_std,
                length=mean_lc_r_hack.shape[0],
                markevery=100,
                xlab='Sample size',
                ylab='MAE',
                lim=[5, 20],
                xlim=[100,1500],
                file='MAE_LCR4')
```


MAE
Sample size
training MAE
test MAE