Initialization settings - Load the packages

Load the required packages and define the function to fix the random seed

In [1]:

```
# The initialization settings - Load the required packages
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import tensorflow as tf
import tensorflow_datasets as tfds
import tensorflow_probability as tfp
import tensorflow.keras as tkeras
from sklearn.decomposition import PCA
from sklearn.preprocessing import OneHotEncoder
from sklearn.neighbors import LocalOutlierFactor
from sklearn.cluster import DBSCAN
from statsmodels.tsa.seasonal import seasonal_decompose
import random

# Note that 'edward2' is not a built-in Python package of Kaggle.
# When you first load it, you need to install it using 'pip'.
import os
os.system('pip install edward2')
import edward2 as ed2

# Define the function to fix the random seed
def set_seed(seed = 0):
    random.seed(seed)
    os.environ['PYTHONHASHSEED'] = str(seed)
    np.random.seed(seed)
    tf.random.set_seed(seed)
```

Part 1 - The exploration on the Wine data set

Load the Wine data set
You first need to upload this data set to the following path on Kaggle:
'../input/wine-dataset/wine.csv'

Perform some initial analyses on Wine data set

In [2]:

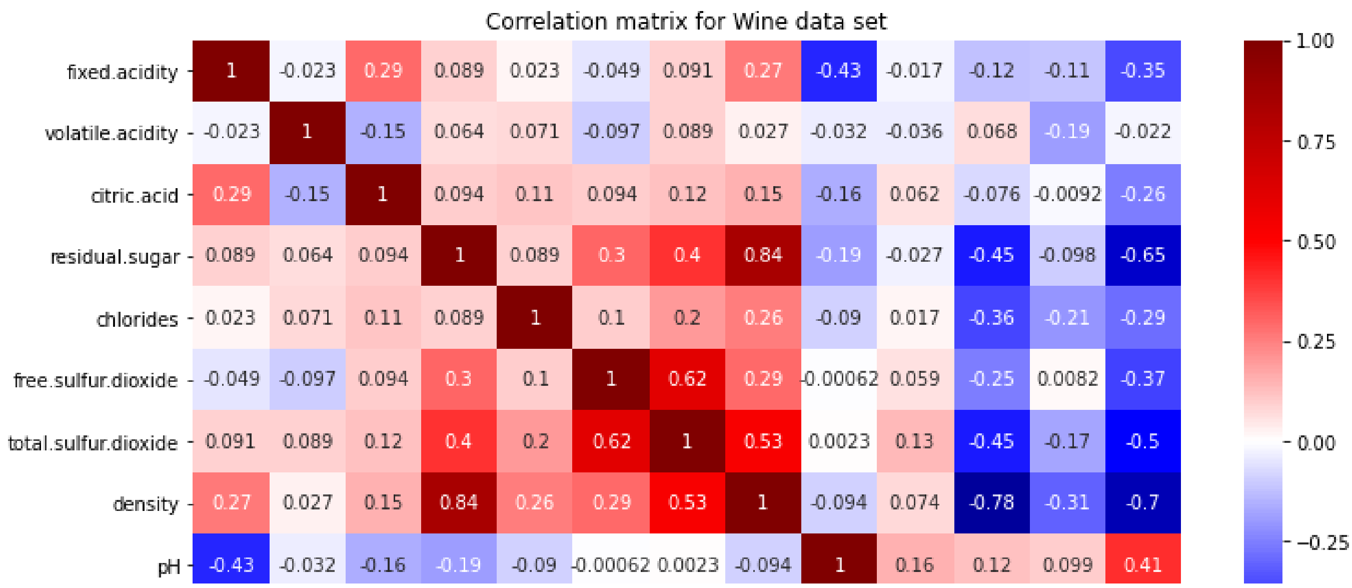
```
# Load the Wine data set
# You first need to upload this data set to the following path:
# '../input/wine-dataset/wine.csv'
wine = pd.read_csv('../input/wine-dataset/wine.csv', sep = ',')
dataset_size = len(wine)

# Fix the random seed
set_seed(seed = 60)

# Some initial analyses on Wine data set
print(wine.info()); display(wine.describe())
plt.figure(figsize = (12, 8))
sns.heatmap(wine.corr(), annot = True, cmap = 'seismic',
            vmin = -1, vmax = 1, center = 0)
plt.title('Correlation matrix for Wine data set')
display(wine[['quality']].join(pd.DataFrame({'count' : [1 for i in range(dataset_size)]}
)).\
    groupby('quality').count())
```

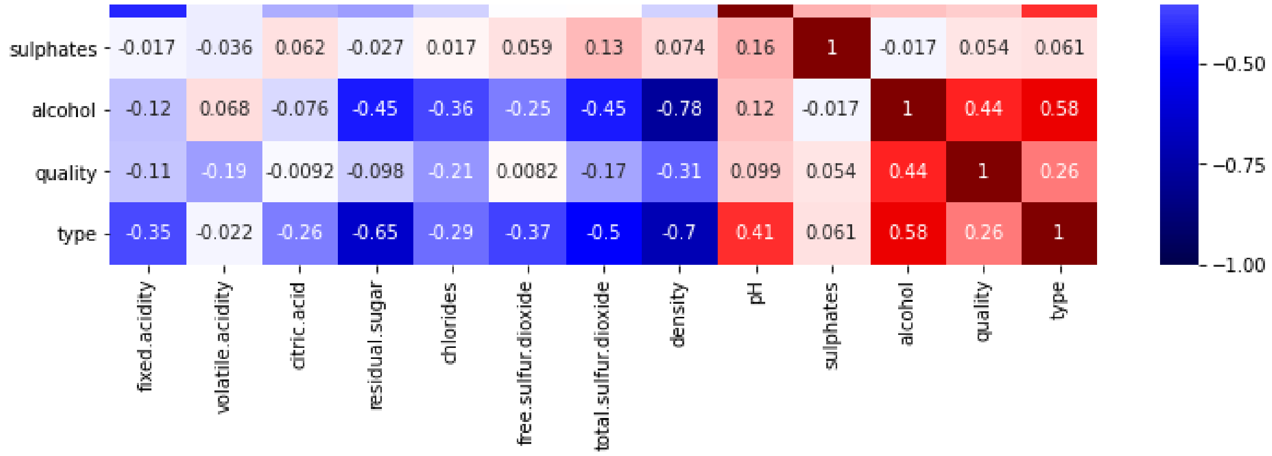
```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 4898 entries, 0 to 4897
```

```
RangeIndex: 4898 entries, 0 to 4897
Data columns (total 13 columns):
 #   Column                Non-Null Count  Dtype  
---  ------                --------------  -----  
 0   fixed.acidity         4898 non-null   float64
 1   volatile.acidity      4898 non-null   float64
 2   citric.acid           4898 non-null   float64
 3   residual.sugar        4898 non-null   float64
 4   chlorides             4898 non-null   float64
 5   free.sulfur.dioxide   4898 non-null   float64
 6   total.sulfur.dioxide  4898 non-null   float64
 7   density               4898 non-null   float64
 8   pH                    4898 non-null   float64
 9   sulphates             4898 non-null   float64
 10  alcohol               4898 non-null   float64
 11  quality               4898 non-null   int64  
 12  type                  4898 non-null   int64  
dtypes: float64(11), int64(2)
memory usage: 497.6 KB
None
```

	fixed.acidity	volatile.acidity	citric.acid	residual.sugar	chlorides	free.sulfur.dioxide	total.sulfur.dioxide	densit
count	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.00000
mean	6.854788	0.278241	0.334192	6.391415	0.045772	35.308085	138.360657	0.99402
std	0.843868	0.100795	0.121020	5.072058	0.021848	17.007137	42.498065	0.00299
min	3.800000	0.080000	0.000000	0.600000	0.009000	2.000000	9.000000	0.98711
25%	6.300000	0.210000	0.270000	1.700000	0.036000	23.000000	108.000000	0.99172
50%	6.800000	0.260000	0.320000	5.200000	0.043000	34.000000	134.000000	0.99374
75%	7.300000	0.320000	0.390000	9.900000	0.050000	46.000000	167.000000	0.99610
max	14.200000	1.100000	1.660000	65.800000	0.346000	289.000000	440.000000	1.03898

	count
quality	
3	20
4	163
5	1457
6	2198
7	880
8	175
9	5





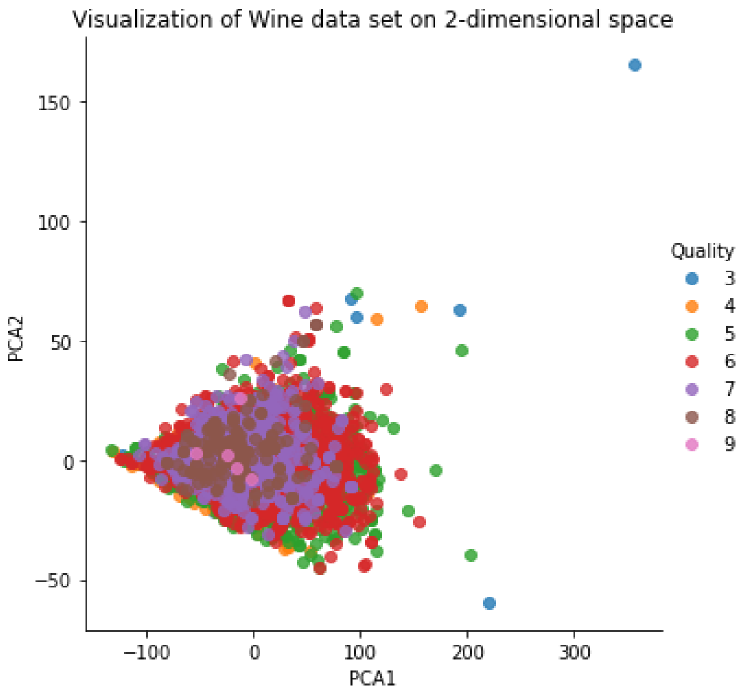
Visualize the Wine data set on 2-dimensional space using the Principal Component Analysis (PCA) technique

In [3]:

```
# In order to visualize the Wine data set, I use Principal Component Analysis
# (PCA) technique to reduce the dimension of the features of this data set.
model_dimredu = PCA(n_components = 2)
wine_features = wine.drop(['quality'], 1)
model_dimredu.fit(wine_features)
wine_features_2D = model_dimredu.transform(wine_features)

# I visualize the Wine data set on 2-dimensional space, with the
# data points classified by wine quality.
wine_dimredu = pd.concat(
    [pd.DataFrame(wine_features_2D, columns = ['PCA1', 'PCA2']),\
    wine[['quality']].rename(columns = {'quality' : 'Quality'})], axis = 1)
sns.lmplot(x = 'PCA1', y = 'PCA2', hue = 'Quality', data = wine_dimredu, fit_reg = False
)
plt.title('Visualization of Wine data set on 2-dimensional space')
```

Out[3]:

```
Text(0.5, 1.0, 'Visualization of Wine data set on 2-dimensional space')
```



Prepare the data used to train the model and split them into train, validation and test set

In [4]:

```
# Prepare the data used to train the model
# Prepare the features and target of the Wine data set separately, convert the
# data set to "tensorflow.dataset" type and convert "wine quality" to "float" type
```

```
features = tf.constant(wine.drop(['quality'], 1))
labels = tf.constant(wine[['quality']])
wine_tfds = tf.data.Dataset.from_tensor_slices((features, labels)).\
    map(lambda x, y: (x, tf.cast(y, tf.float64))).\
    shuffle(buffer_size = dataset_size).prefetch(buffer_size = dataset_size)

# Split the data set into train, validation and test set, and batch each set
train_size = round(dataset_size*0.8)
validation_size = round(dataset_size*0.1)
test_size = dataset_size - train_size - validation_size
batch_size = 256
wine_train = wine_tfds.take(train_size).batch(batch_size)
wine_validation = wine_tfds.skip(train_size).take(validation_size).batch(validation_size)
wine_test = wine_tfds.skip(train_size + validation_size).batch(test_size)
```

Define the prior and variational posterior of network weight parameters and define the negative log-likelihood function of the model

In [5]:

```
# Define the prior weight distributions as independent standard normal distributions
def prior(kernel_size, bias_size, dtype = None):
    n = kernel_size + bias_size
    return tkeras.Sequential([
        tfp.layers.DistributionLambda(
            lambda t: tfp.distributions.MultivariateNormalDiag(
                loc = tf.zeros(n), scale_diag = tf.ones(n))
        )
    ])

# Define the variational posterior weight distribution as multivariate Gaussian distribut
ion
# The trainable parameters for this distribution are the means, variances, and covariance
s.
def posterior(kernel_size, bias_size, dtype = None):
    n = kernel_size + bias_size
    return tkeras.Sequential([
               tfp.layers.VariableLayer(
                   tfp.layers.MultivariateNormalTriL.params_size(n), dtype = dtype
               ),
               tfp.layers.MultivariateNormalTriL(n),
           ])

# Define the negative log-likelihood function of the model
def negative_log_likelihood(y_true, y_pred):
    return -y_pred.log_prob(y_true)
```

Construct and train the Bayesian neural network (BNN) model

In [ ]:

```
# Specify some model parameters
kl_loss_weight = 1/train_size
learning_rate = 0.001
num_epochs = 1000

# Construct the Bayesian neural network model with two hidden layers
wine_model = tkeras.Sequential([
    tkeras.layers.Input(shape = (12,)),
    tkeras.layers.BatchNormalization(),
    tfp.layers.DenseVariational(
        units = 8, make_posterior_fn = posterior,
        make_prior_fn = prior, kl_weight = kl_loss_weight,
        activation = 'sigmoid'
    ),
    tfp.layers.DenseVariational(
        units = 8, make_posterior_fn = posterior,
        make_prior_fn = prior, kl_weight = kl_loss_weight,
        activation = 'sigmoid'
    ),
```

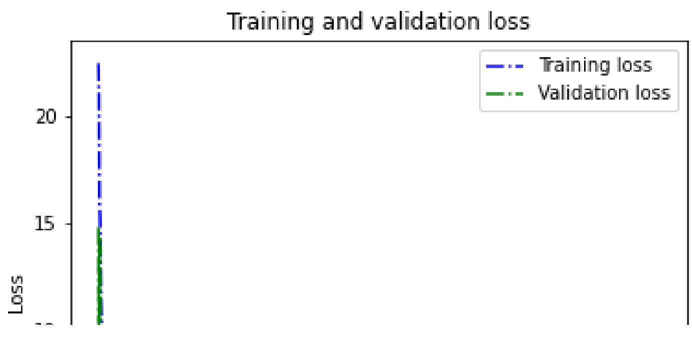
```
    tkeras.layers.Dense(units = 2),
    tfp.layers.IndependentNormal(1)
])

# View the structure of the model
wine_model.summary()

# Compile the constructed Bayesian neural network
# We take the negative Evidence Lower Bound (-ELBO) as the loss function,
# and use the RMSprop optimizer with learning rate being equal to 0.001 to
# minimize the loss function, and use Mean Square Error (MSE) as the metric
# to evaluate the accuracy of the model.
wine_model.compile(
    optimizer = tkeras.optimizers.RMSprop(learning_rate = learning_rate),
    loss = negative_log_likelihood,
    metrics = [tkeras.metrics.mean_squared_error]
)

# Fit the constructed Bayesian neural network with data
wine_fit = wine_model.fit(x = wine_train, epochs = num_epochs,
                          validation_data = wine_validation)
```

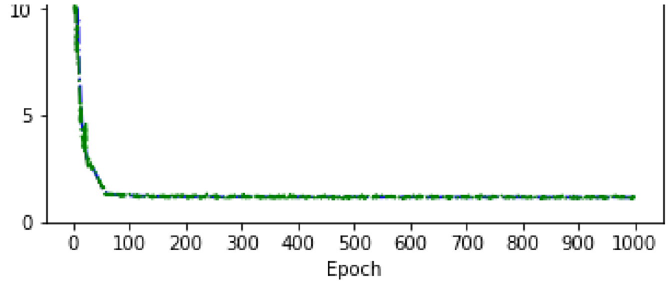
Draw the trend of the loss and the MSE on the train and validation set during the training process respectively

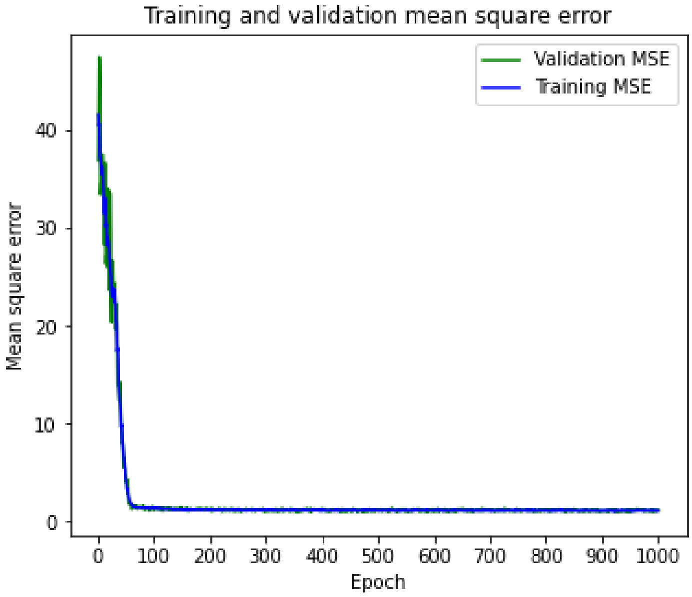
In [7]:

```
# Draw the trend of the loss and the MSE on the train and
# validation set during the training process respectively

# Prepare the data
train_loss = wine_fit.history['loss']
val_loss = wine_fit.history['val_loss']
train_eva = wine_fit.history['mean_squared_error']
val_eva = wine_fit.history['val_mean_squared_error']
epochs = range(1, num_epochs + 1)

# The trend of loss on the train and validation set
fig1 = plt.figure(figsize = (6, 5)); ax1 = plt.axes()
ax1.plot(epochs, train_loss, 'b-.', label = 'Training loss')
ax1.plot(epochs, val_loss, 'g-.', label = 'Validation loss')
ax1.xaxis.set_major_locator(plt.MultipleLocator(100))
ax1.set(xlabel = 'Epoch', ylabel = 'Loss',
        title = 'Training and validation loss')
ax1.legend()

# The trend of the metric (MSE) on the train and validation set
fig2 = plt.figure(figsize = (6, 5)); ax2 = plt.axes()
ax2.plot(epochs, val_eva, 'g-', label = 'Validation MSE')
ax2.plot(epochs, train_eva, 'b-', label = 'Training MSE')
ax2.xaxis.set_major_locator(plt.MultipleLocator(100))
ax2.set(xlabel = 'Epoch', ylabel = 'Mean square error',
        title = 'Training and validation mean square error')
ax2.legend()

# Evaluate the trained model on both train set and test set respectively
print(wine_model.evaluate(wine_train, verbose = 0))
print(wine_model.evaluate(wine_test, verbose = 0))
```

```
[1.1512471437454224, 1.1381399631500244]
[1.1099435091018677, 1.0951550006866455]
```







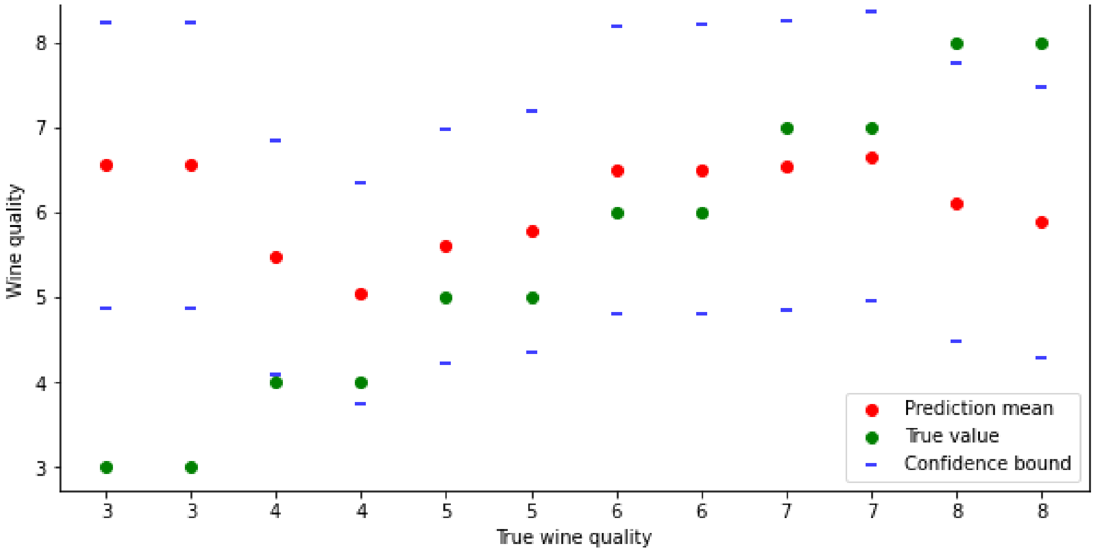
I take 12 samples from the test set, two samples per quality level (from 3 to 8). Then, I construct and visualize the 95% confidence intervals for the predictions of these selected samples.

In [8]:

```
# Take 12 samples from the test set, two samples per quality level (from 3 to 8)
features_exa, targets_exa = list(wine_test)[0]
features_exa = features_exa.numpy()
targets_exa = targets_exa.numpy()[:, 0]
sample_ind = np.array([])
for k in range(3, 9):
    choice = np.random.choice(np.where(targets_exa == k)[0], size = 2)
    sample_ind = np.concatenate([sample_ind, choice])
examples = features_exa[sample_ind.astype('int'), :]
labels_exa = targets_exa[sample_ind.astype('int')]

# Compare the prediction means with the true labels
examples_mean = wine_model(examples).mean().numpy()
examples_std = wine_model(examples).stddev().numpy()

# Construct and visualize the 95% confidence intervals for the predictions
plt.figure(figsize = (10, 5))
index = range(1, 13)
quality = np.concatenate(np.array([[k, k] for k in range(3, 9)]))
plt.scatter(index, examples_mean, color = 'red', label = 'Prediction mean')
plt.scatter(index, labels_exa, color = 'green', label = 'True value')
plt.scatter(index, examples_mean + 1.96*examples_std,
            color = 'blue', marker = '_', label = 'Confidence bound')
plt.scatter(index, examples_mean - 1.96*examples_std,
            color = 'blue', marker = '_')
plt.xlabel('True wine quality'); plt.ylabel('Wine quality')
plt.xticks(ticks = index, labels = quality)
plt.title('The 95% confidence intervals for the predictions of twelve selected samples')
plt.legend()
```

Out[8]:

```
<matplotlib.legend.Legend at 0x7f22401a4bd0>
```



Clear the model and re-train the model with the whole data set

In [ ]:

```
# Clear the model and re-train the model with the whole data set

# Update the weight for the KL divergence loss between
# the surrogate posterior and weight prior
kl_loss_weight = 1/dataset_size

# Clear the model
wine_model = tkeras.Sequential([
    tkeras.layers.Input(shape = (12,)),
    tkeras.layers.BatchNormalization(),
    tfp.layers.DenseVariational(
        units = 8, make_posterior_fn = posterior,
        make_prior_fn = prior, kl_weight = kl_loss_weight,
        activation = 'sigmoid'
    ),
    tfp.layers.DenseVariational(
        units = 8, make_posterior_fn = posterior,
        make_prior_fn = prior, kl_weight = kl_loss_weight,
        activation = 'sigmoid'
    ),
    tkeras.layers.Dense(units = 2),
    tfp.layers.IndependentNormal(1)
])

# Re-compile the model with the same settings
wine_model.compile(
    optimizer = tkeras.optimizers.RMSprop(learning_rate = learning_rate),
    loss = negative_log_likelihood,
    metrics = [tkeras.metrics.mean_squared_error]
)

# Re-fit the model with the whole data set
wine_model.fit(x = wine_tfds.batch(batch_size), epochs = num_epochs)
```

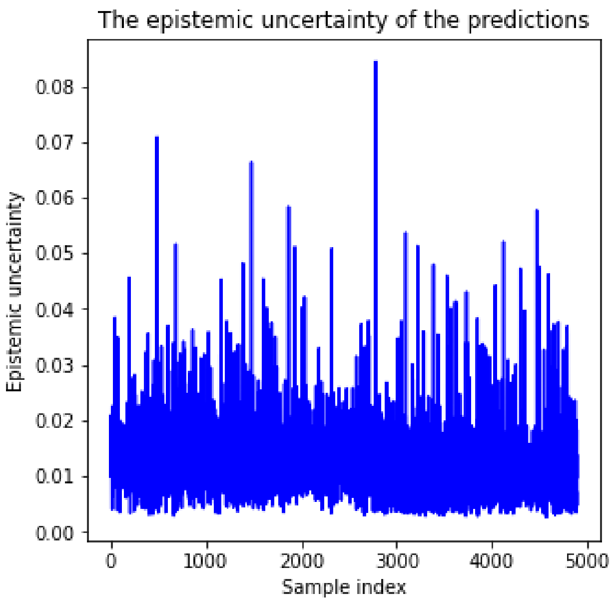
Quantify and plot all kinds of uncertainties of the predictions

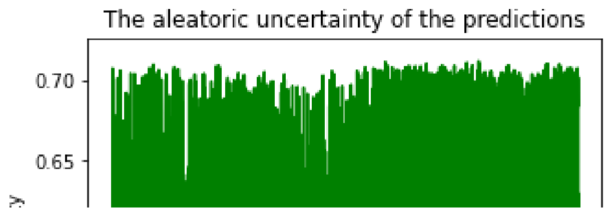
In [10]:

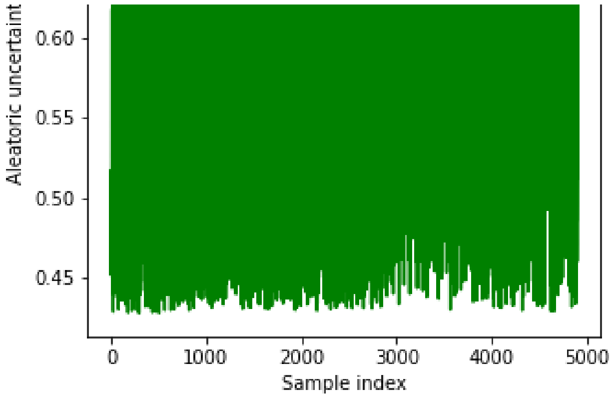
```
# Quantify all kinds of uncertainties of the predictions
N = 1000; records = np.zeros((N, dataset_size, 3))
for i in range(N):
    records[i, :, 0] = wine_model(features).mean().numpy()[:, 0]
    records[i, :, 1] = wine_model(features).variance().numpy()[:, 0]
    records[i, :, 2] = ((wine_model(features).mean().numpy() - labels.numpy())**2)[:, 0]
epistemic = np.var(records[:, :, 0], axis = 0)
aleatoric = np.mean(records[:, :, 1], axis = 0)
misspecification = np.mean(records[:, :, 2], axis = 0)
```

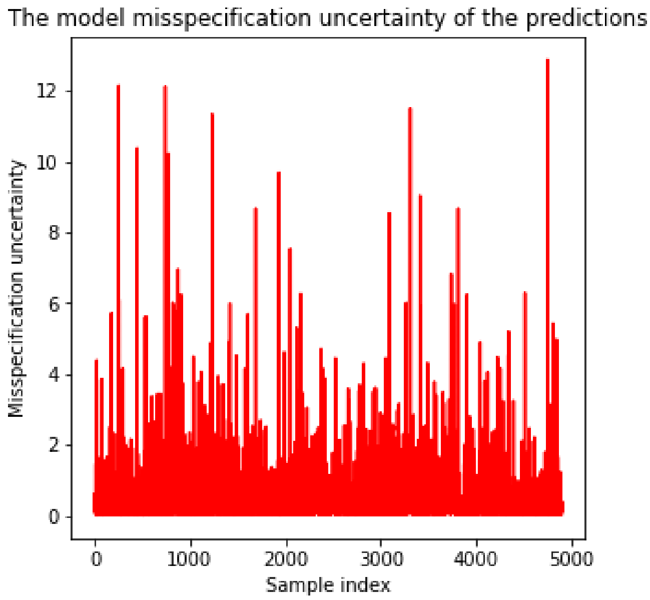
```
P = 1; Q = 1; R = 1
comp_uncer = P*epistemic + Q*aleatoric + R*misspecification

# Plot all kinds of uncertainties
X = range(1, dataset_size + 1)

# Plot the epistemic uncertainty
plt.figure(figsize = (5, 5))
plt.plot(X, epistemic, 'b-')
plt.xlabel('Sample index')
plt.ylabel('Epistemic uncertainty')
plt.title('The epistemic uncertainty of the predictions')

# Plot the aleatoric uncertainty
plt.figure(figsize = (5, 5))
plt.plot(X, aleatoric, 'g-')
plt.xlabel('Sample index')
plt.ylabel('Aleatoric uncertainty')
plt.title('The aleatoric uncertainty of the predictions')

# Plot the model misspecification uncertainty
plt.figure(figsize = (5, 5))
plt.plot(X, misspecification, 'r-')
plt.xlabel('Sample index')
plt.ylabel('Misspecification uncertainty')
plt.title('The model misspecification uncertainty of the predictions')

# Plot the total prediction uncertainty
plt.figure(figsize = (10, 5))
plt.plot(X, comp_uncer, color = 'darkviolet')
plt.xlabel('Sample index')
plt.ylabel('Prediction uncertainty')
plt.title('The complete measurement of prediction uncertainty')
threshold = 3
plt.axhline(threshold, color = 'red')

# Record the information about the index of outliers
index = (comp_uncer > threshold).astype('int').tolist()
wine_BNN = wine_dimredu.join(pd.DataFrame(index, columns = ['indicator'])).\
                        join(pd.DataFrame(comp_uncer, columns = ['uncertainty']))
print(np.mean(index)); print(np.sum(index))
```

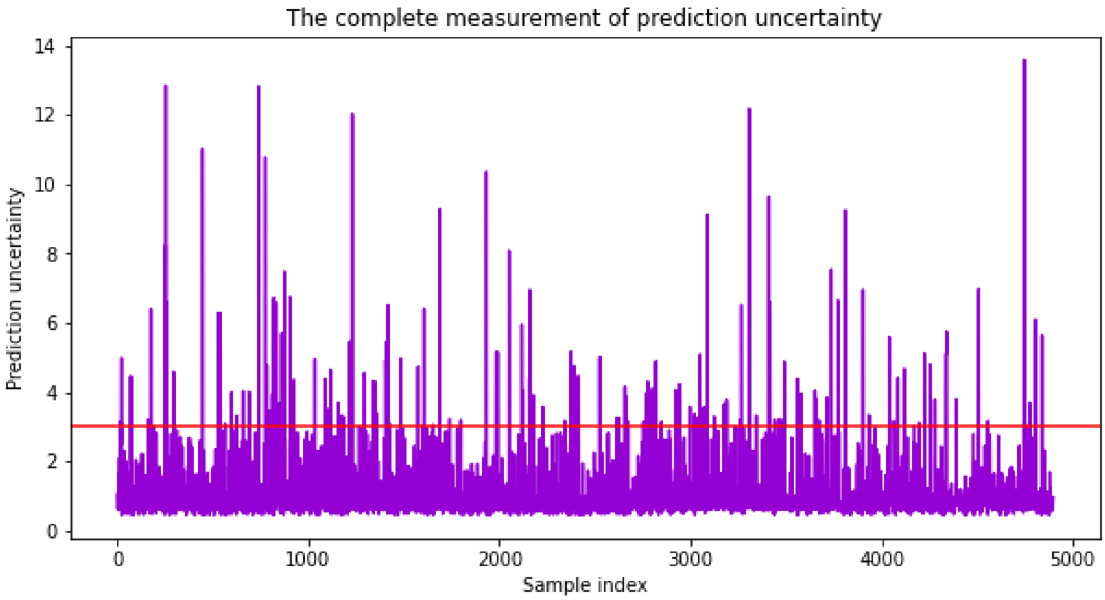
```
0.04062882809309922
199
```











Perform the Local Outlier Factor (LOF) method and DBSCAN method on Wine data set

In [11]:

```
# Perform the Local Outlier Factor (LOF) method on Wine data set
Lof = LocalOutlierFactor()
Lof_pre = Lof.fit_predict(wine)
Lof_fac = Lof.negative_outlier_factor_
wine_LOF = wine_dimredu.join(pd.DataFrame(Lof_pre, columns = ['indicator'])).\
                        join(pd.DataFrame(Lof_fac, columns = ['factor']))

# Perform the DBSCAN method on Wine data set
DBSCAN_model = DBSCAN(eps = 8, min_samples = 5)
DBSCAN_fit = DBSCAN_model.fit(wine)
DBSCAN_pre = DBSCAN_fit.labels_
```

```
DBSCAN_noise = (DBSCAN_pre == -1).astype('int')
wine_DBSCAN = wine_dimredu.join(pd.DataFrame(DBSCAN_noise, columns = ['indicator']))
```

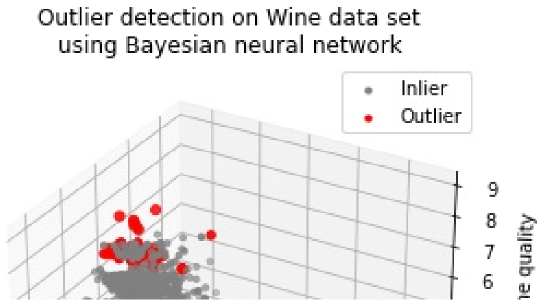
Visualize the results of outlier detection using BNN, LOF and DBSCAN method respectively

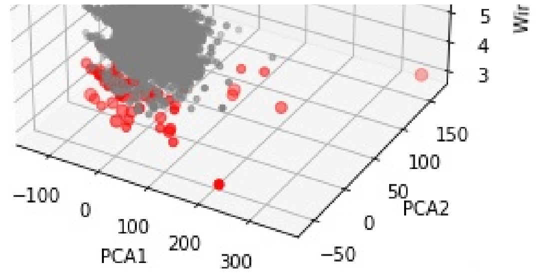
In [12]:

```
# Visualize the effects of the three outlier detection methods on Wine data set

# The visualization of the effect of Bayesian neural network
plt.figure(figsize = (5, 5))
ax1 = plt.axes(projection = '3d')
uncer_outlier = wine_BNN['uncertainty'][wine_BNN['indicator'] == 1]
ax1.scatter3D(wine_BNN['PCA1'][wine_BNN['indicator'] == 0],
              wine_BNN['PCA2'][wine_BNN['indicator'] == 0],
              wine_BNN['Quality'][wine_BNN['indicator'] == 0],
              c = 'gray', s = 10, label = 'Inlier')
ax1.scatter3D(wine_BNN['PCA1'][wine_BNN['indicator'] == 1],
              wine_BNN['PCA2'][wine_BNN['indicator'] == 1],
              wine_BNN['Quality'][wine_BNN['indicator'] == 1],
              c = 'red', s = 10 + 2.5*uncer_outlier)
ax1.scatter3D([], [], [], c = 'red', s = 10, label = 'Outlier')
ax1.set(xlabel = 'PCA1', ylabel = 'PCA2', zlabel = 'Wine quality',
        title = 'Outlier detection on Wine data set\nusing Bayesian neural network')
plt.legend()

# The visualization of the effect of Local Outlier Factor method
plt.figure(figsize = (5, 5))
ax2 = plt.axes(projection = '3d')
ax2.scatter3D(wine_LOF['PCA1'][wine_LOF['indicator'] == 1],
              wine_LOF['PCA2'][wine_LOF['indicator'] == 1],
              wine_LOF['Quality'][wine_LOF['indicator'] == 1],
              c = 'gray', s = 10, label = 'Inlier')
LOF_outlier = wine_LOF['factor'][wine_LOF['indicator'] == -1]
ax2.scatter3D(wine_LOF['PCA1'][wine_LOF['indicator'] == -1],
              wine_LOF['PCA2'][wine_LOF['indicator'] == -1],
              wine_LOF['Quality'][wine_LOF['indicator'] == -1],
              c = 'red', s = 10 - 4*LOF_outlier)
ax2.scatter3D([], [], [], c = 'red', s = 10, label = 'Outlier')
ax2.set(xlabel = 'PCA1', ylabel = 'PCA2', zlabel = 'Wine quality',
        title = 'Outlier detection on Wine data set\nusing Local Outlier Factor method')
plt.legend()

# The visualization of the effect of DBSCAN method
plt.figure(figsize = (5, 5))
ax3 = plt.axes(projection = '3d')
ax3.scatter3D(wine_DBSCAN['PCA1'][wine_DBSCAN['indicator'] == 0],
              wine_DBSCAN['PCA2'][wine_DBSCAN['indicator'] == 0],
              wine_DBSCAN['Quality'][wine_DBSCAN['indicator'] == 0],
              c = 'gray', s = 10, label = 'Inlier')
ax3.scatter3D(wine_DBSCAN['PCA1'][wine_DBSCAN['indicator'] == 1],
              wine_DBSCAN['PCA2'][wine_DBSCAN['indicator'] == 1],
              wine_DBSCAN['Quality'][wine_DBSCAN['indicator'] == 1],
              c = 'red', s = 10, label = 'Outlier')
ax3.set(xlabel = 'PCA1', ylabel = 'PCA2', zlabel = 'Wine quality',
        title = 'Outlier detection on Wine data set\nusing DBSCAN method')
plt.legend()
```

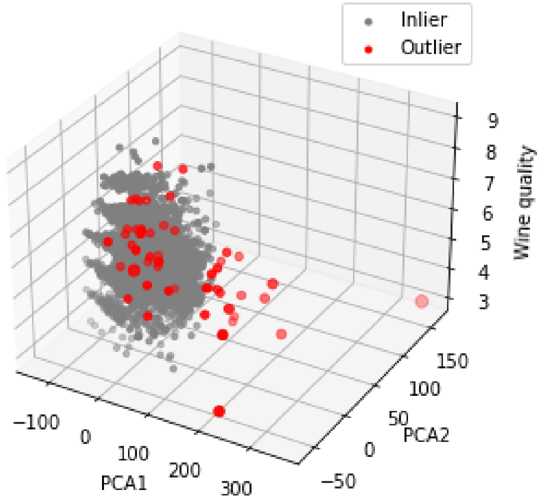
Out[12]:

```
<matplotlib.legend.Legend at 0x7f22140bf690>
```

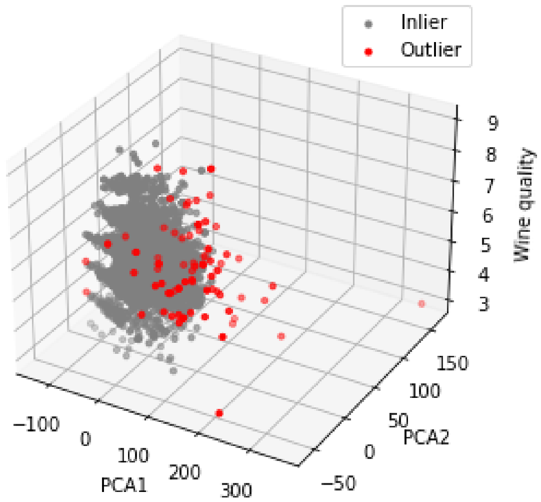




Outlier detection on Wine data set
using Local Outlier Factor method



Outlier detection on Wine data set
using DBSCAN method



Part 2 - The exploration on the MNIST data set

Load the MNIST data set
You first need to upload this data set to the following path on Kaggle:
'../input/mnist-dataset/mnist.csv'

Perform some initial analyses on MNIST data set

In [13]:

```
# Load the MNIST data set and adjust the column name
# You first need to upload this data set to the following path:
# '../input/mnist-dataset/mnist.csv'
mnist = pd.read_csv('../input/mnist-dataset/mnist.csv', sep = ',')
mnist.rename(columns = {'Unnamed: 0' : 'index_ori'}, inplace = True)
mnist_data = mnist.drop(['index_ori'], 1)

# Fix the random seed
set_seed(seed = 200)
```

```python
# Some initial analyses on the MNIST data set
dataset_size = len(mnist)
print(mnist.info()); display(mnist.describe())
display(mnist[['label']].join(pd.DataFrame({'count' : [1 for i in range(dataset_size)]})
).\
    groupby('label').count())
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 17280 entries, 0 to 17279
Columns: 786 entries, index_ori to pixel783
dtypes: float64(784), int64(2)
memory usage: 103.6 MB
None
```

	index_ori	label	pixel0	pixel1	pixel2	pixel3	pixel4	pixel5	pixel6	pixel7	...	pixel774
count	17280.000000	17280.000000	17280.0	17280.0	17280.0	17280.0	17280.0	17280.0	17280.0	17280.0	...	17280.000000
mean	21083.968113	3.934896	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.001844
std	12125.338906	3.509446	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.035979
min	0.000000	0.000000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.000000
25%	10597.750000	1.000000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.000000
50%	21117.000000	1.000000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.000000
75%	31644.000000	7.000000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.000000
max	41997.000000	8.000000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.996078

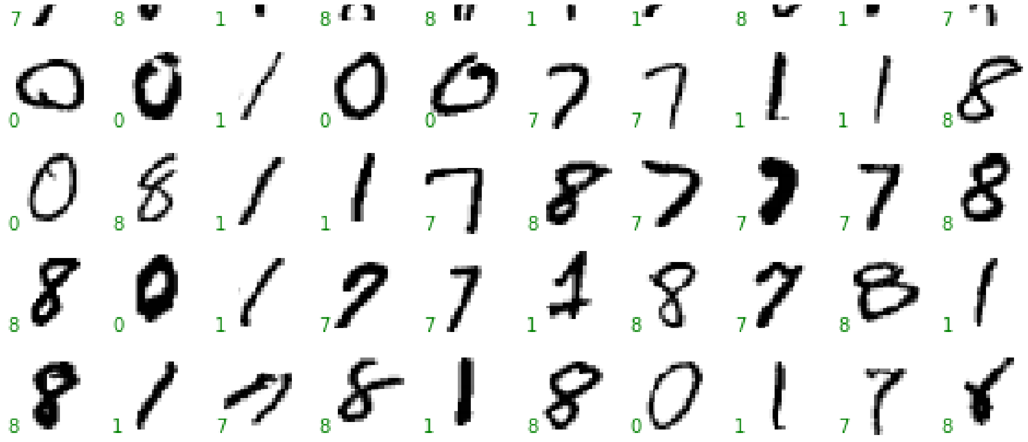
8 rows × 786 columns

	count
label	
0	4132
1	4684
7	4401
8	4063

I randomly take 50 samples from MNIST data set and visualize these digits.

In [14]:

```python
# Randomly take some samples from MNIST data set and visualize these digits
n_examples = 50
examples = np.random.permutation(mnist)[:n_examples, :]
features_exa = examples[:, 2:].reshape(n_examples, 28, 28)
labels_exa = examples[:, 1].astype('int')

columns = 10; rows = int(n_examples/columns)
figs, axes = plt.subplots(rows, columns, figsize = (columns, rows),
                          subplot_kw = {'xticks':[], 'yticks':[]},
                          gridspec_kw = dict(hspace = 0.1, wspace = 0.1))
plt.suptitle('Display of some handwritten digits in MNIST data set')
for i, ax in enumerate(axes.flat):
    ax.imshow(features_exa[i], cmap = 'binary', interpolation = 'nearest')
    ax.text(0.05, 0.05, str(labels_exa[i]), transform = ax.transAxes, color = 'green')
    ax.spines['top'].set_visible(False)
    ax.spines['right'].set_visible(False)
    ax.spines['bottom'].set_visible(False)
    ax.spines['left'].set_visible(False)
```



Prepare the data used to train the model and split them into train, validation and test set

In [15]:

```
# Prepare the data used to train the model
# Prepare the features and target of MNIST data set separately, and
# convert the data set to "tensorflow.dataset" type
mnist_onehot = OneHotEncoder()
mnist_onehot.fit(mnist_data[['label']].values)
labels = mnist_onehot.transform(mnist_data[['label']].values).A
features = tf.constant(mnist_data.loc[:, 'pixel0':'pixel783'].\
                       values.reshape(dataset_size, 28, 28, 1))
labels = tf.constant(labels)
mnist_tfds = tf.data.Dataset.from_tensor_slices((features, labels)).\
    shuffle(buffer_size = dataset_size).prefetch(buffer_size = dataset_size)

# Split the data set into train, validation and test set
train_size = round(dataset_size*0.85)
validation_size = round(dataset_size*0.075)
test_size = dataset_size - train_size - validation_size
mnist_train = mnist_tfds.take(train_size).batch(train_size)
mnist_validation = mnist_tfds.skip(train_size).take(validation_size).batch(validation_siz
e)
mnist_test = mnist_tfds.skip(train_size + validation_size).batch(test_size)
```

Construct and train the Bayesian convolutional neural network (BCNN) model

In [ ]:

```
# Specify some model parameters
learning_rate = 0.002
num_epochs = 2000

# Define the loss function
# We still use the negative Evidence Lower Bound as the loss function
def negative_ELBO(label_true, label_pred):
    neg_log_likelihood = -tf.reduce_sum(label_pred.log_prob(label_true))
    kl = sum(mnist_model.losses)
    return neg_log_likelihood + kl/train_size

# Construct the Bayesian convolutional neural network model
mnist_model = tkeras.Sequential([
    tkeras.layers.Input(shape = (28, 28, 1)),
    tfp.layers.Convolution2DFlipout(filters = 4, kernel_size = (5, 5),
                                    padding = "SAME", activation = 'relu'),
    tkeras.layers.MaxPooling2D(pool_size = (2, 2), strides = (2, 2)),
    tfp.layers.Convolution2DFlipout(filters = 8, kernel_size = (5, 5),
                                    padding = "SAME", activation = 'relu'),
    tkeras.layers.MaxPooling2D(pool_size = (2, 2), strides = (2, 2)),
    tfp.layers.Convolution2DFlipout(filters = 16, kernel_size = (5, 5),
                                    padding = "SAME", activation = 'relu'),
    tkeras.layers.Flatten(),
    tkeras.layers.Dropout(0.5),
    tfp.layers.DenseFlipout(units = 8, activation = 'relu'),
```

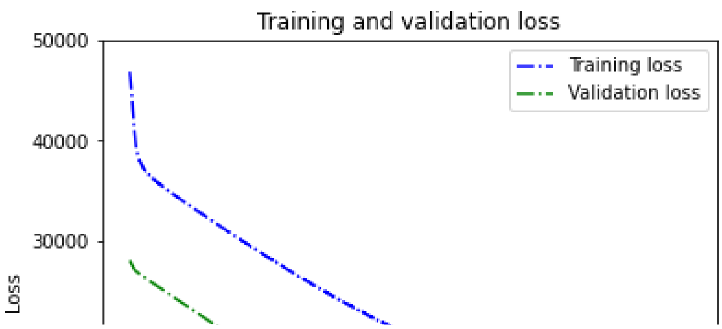
```
    tkeras.layers.Dense(units = 4, activation = 'softmax'),
    tfp.layers.OneHotCategorical(event_size = 4,
                                 convert_to_tensor_fn = tfp.distributions.Distribution.m
ode)
])

# View the structure of the model
mnist_model.summary()

# Compile the constructed Bayesian convolutional neural network
# I use the Adam optimizer with learning rate being equal to 0.002 to minimize the
# loss function, and use the classification accuracy to evaluate the model accuracy.
mnist_model.compile(
    optimizer = tkeras.optimizers.Adam(learning_rate = learning_rate),
    loss = negative_ELBO,
    metrics = [tkeras.metrics.categorical_accuracy]
)

# Fit the constructed Bayesian convolutional neural network with data
mnist_fit = mnist_model.fit(x = mnist_train, epochs = num_epochs,
                            validation_data = mnist_validation)
```

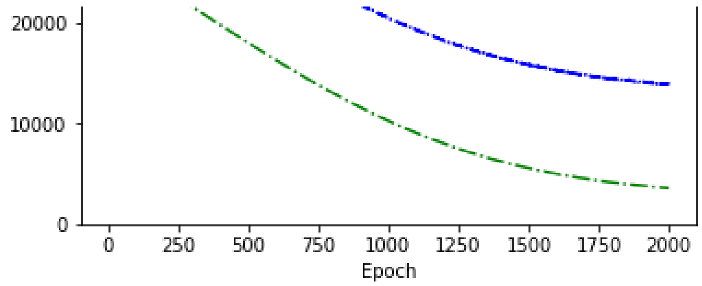
Draw the trend of the loss and the MSE on the train and validation set during the training process respectively

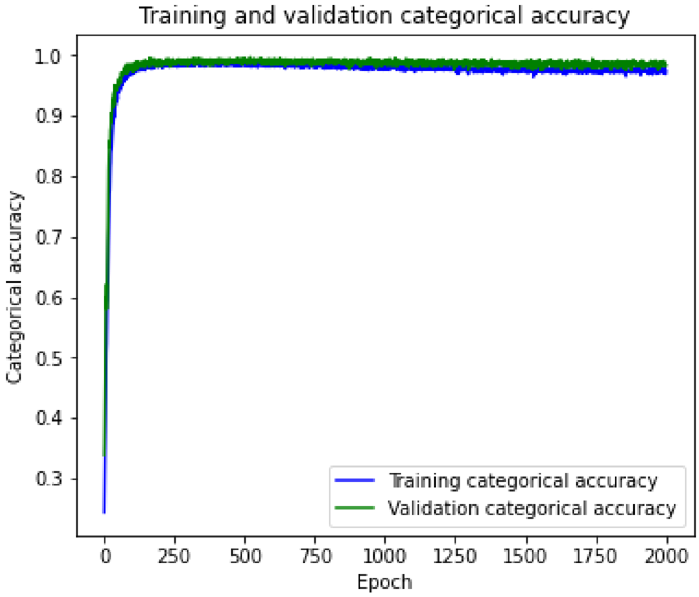
In [17]:

```
# Draw the trend of the loss and the classification accuracy on the
# train and validation set during the training process respectively

# Prepare the data
train_loss = mnist_fit.history['loss']
val_loss = mnist_fit.history['val_loss']
train_eva = mnist_fit.history['categorical_accuracy']
val_eva = mnist_fit.history['val_categorical_accuracy']
epochs = range(1, num_epochs + 1)

# The trend of loss on the train and validation set
fig1 = plt.figure(figsize = (6, 5)); ax1 = plt.axes()
ax1.plot(epochs, train_loss, 'b-.', label = 'Training loss')
ax1.plot(epochs, val_loss, 'g-.', label = 'Validation loss')
ax1.xaxis.set_major_locator(plt.MultipleLocator(250))
ax1.set(xlabel = 'Epoch', ylabel = 'Loss', ylim = (0, 50000),
        title = 'Training and validation loss')
ax1.legend()

# The trend of classification accuracy on the train and validation set
fig2 = plt.figure(figsize = (6, 5)); ax2 = plt.axes()
ax2.plot(epochs, train_eva, 'b-', label = 'Training categorical accuracy')
ax2.plot(epochs, val_eva, 'g-', label = 'Validation categorical accuracy')
ax2.xaxis.set_major_locator(plt.MultipleLocator(250))
ax2.set(xlabel = 'Epoch', ylabel = 'Categorical accuracy',
        title = 'Training and validation categorical accuracy')
ax2.legend()

# Evaluate the trained model on both train set and test set respectively
print(mnist_model.evaluate(mnist_train, verbose = 0))
print(mnist_model.evaluate(mnist_test, verbose = 0))
```

```
[13726.0498046875, 0.9863153696060181]
[3587.12841796875, 0.9845678806304932]
```







Clear the model and re-train the model with the whole data set

In [ ]:

```
# Clear the model and re-train the model with the whole data set

# Re-define the loss function in order to update the weight for the
# KL divergence loss between the surrogate posterior and weight prior
def negative_ELBO(label_true, label_pred):
    neg_log_likelihood = -tf.reduce_sum(label_pred.log_prob(label_true))
    kl = sum(mnist_model.losses)
    return neg_log_likelihood + kl/dataset_size

# Clear the model
mnist_model = tkeras.Sequential([
    tkeras.layers.Input(shape = (28, 28, 1)),
    tfp.layers.Convolution2DFlipout(filters = 4, kernel_size = (5, 5),
                                    padding = "SAME", activation = 'relu'),
    tkeras.layers.MaxPooling2D(pool_size = (2, 2), strides = (2, 2)),
    tfp.layers.Convolution2DFlipout(filters = 8, kernel_size = (5, 5),
                                    padding = "SAME", activation = 'relu'),
    tkeras.layers.MaxPooling2D(pool_size = (2, 2), strides = (2, 2)),
    tfp.layers.Convolution2DFlipout(filters = 16, kernel_size = (5, 5),
                                    padding = "SAME", activation = 'relu'),
    tkeras.layers.Flatten(),
    tkeras.layers.Dropout(0.5),
    tfp.layers.DenseFlipout(units = 8, activation = 'relu'),
    tkeras.layers.Dense(units = 4, activation = 'softmax'),
    tfp.layers.OneHotCategorical(event_size = 4,
                                 convert_to_tensor_fn = tfp.distributions.Distribution.m
ode)
])

# Re-compile the model with the same settings
mnist_model.compile(
    optimizer = tkeras.optimizers.Adam(learning_rate = learning_rate),
    loss = negative_ELBO,
    metrics = [tkeras.metrics.categorical_accuracy]
)
```

```
# Re-fit the model with the whole data set
mnist_model.fit(x = mnist_tfds.batch(dataset_size), epochs = num_epochs)
```

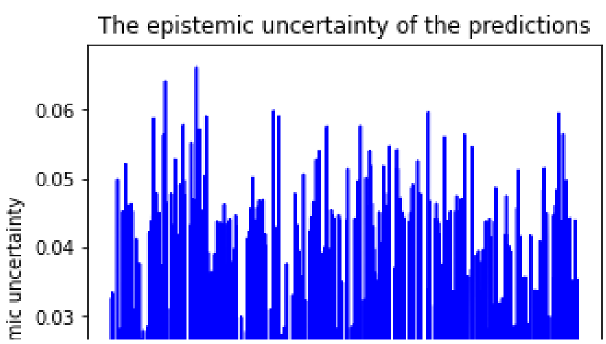
Quantify and plot all kinds of uncertainties of the predictions

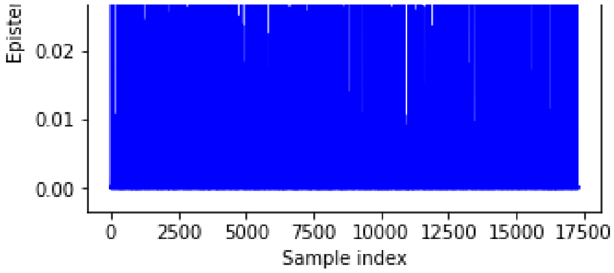
In [19]:

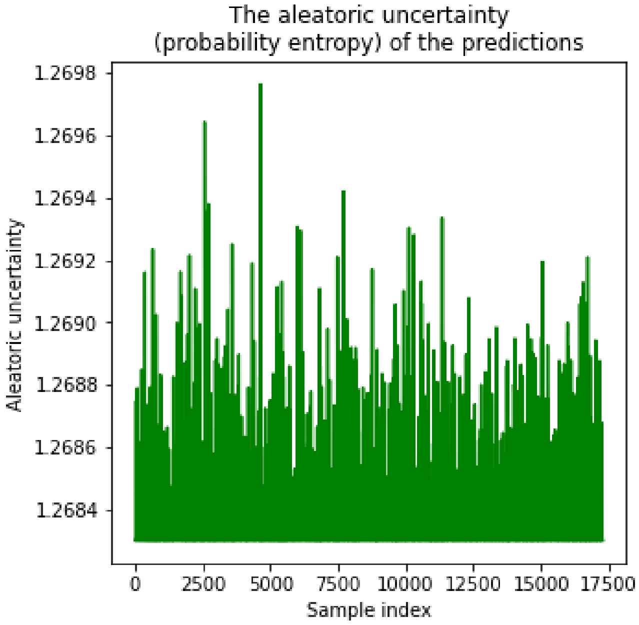
```
# Quantify all kinds of uncertainties of the predictions
N = 1000; records = np.zeros((N, dataset_size, 6))
for i in range(N):
    records[i, :, 0:4] = mnist_model(features).mean().numpy()
    records[i, :, 4] = mnist_model(features).entropy().numpy()
    records[i, :, 5] = -np.sum(np.log(mnist_model(features).mean().numpy())*\
                               labels.numpy(), axis = 1)
epistemic = 0
for i in range(4):
    epistemic += np.var(records[:, :, i], axis = 0)
aleatoric = np.mean(records[:, :, 4], axis = 0)
misspecification = np.mean(records[:, :, 5], axis = 0)
P = 1/np.std(epistemic); Q = 1/np.std(aleatoric); R = 1/np.std(misspecification);
W = -(P*np.min(epistemic) + Q*np.min(aleatoric) + R*np.min(misspecification))
comp_uncer = P*epistemic + Q*aleatoric + R*misspecification + W

# Plot all kinds of uncertainties
X = range(1, dataset_size + 1)

# Plot the epistemic uncertainty
plt.figure(figsize = (5, 5))
plt.plot(X, epistemic, 'b-')
plt.xlabel('Sample index')
plt.ylabel('Epistemic uncertainty')
plt.title('The epistemic uncertainty of the predictions')

# Plot the aleatoric uncertainty (entropy of the probability vector)
plt.figure(figsize = (5, 5))
plt.plot(X, aleatoric, 'g-')
plt.xlabel('Sample index')
plt.ylabel('Aleatoric uncertainty')
plt.title('The aleatoric uncertainty\n(probability entropy) of the predictions')

# Plot the model misspecification uncertainty (cross-entropy of the probability vector)
plt.figure(figsize = (5, 5))
plt.plot(X, misspecification, 'r-')
plt.xlabel('Sample index')
plt.ylabel('Misspecification uncertainty')
plt.title('The model misspecification uncertainty\n(probability' +
          ' cross-entropy) of the predictions')

# Plot the total prediction uncertainty
plt.figure(figsize = (10, 5))
plt.plot(X, comp_uncer, color = 'darkviolet')
plt.xlabel('Sample index')
plt.ylabel('Prediction uncertainty')
plt.title('The complete measurement of prediction uncertainty')
threshold = 15
plt.axhline(threshold, color = 'red')
```

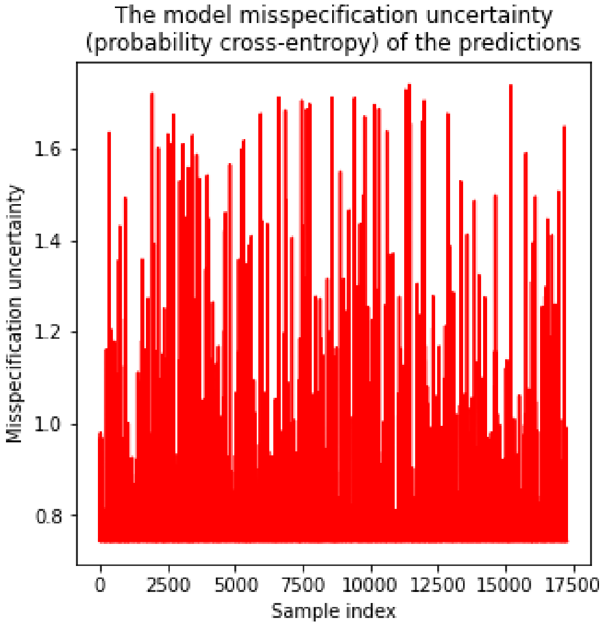
Out[19]:

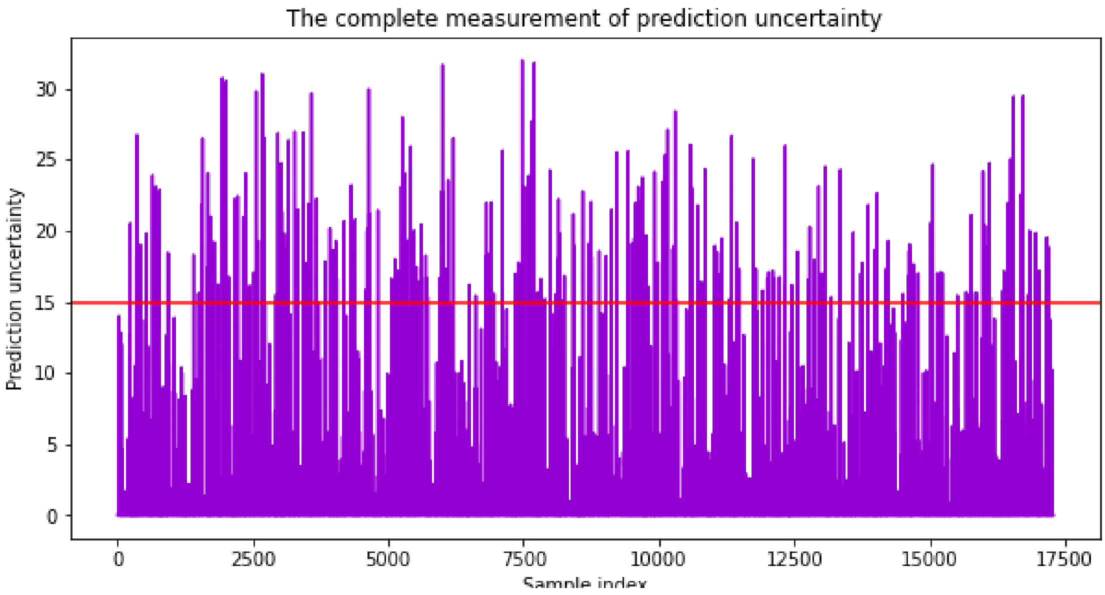
```
<matplotlib.lines.Line2D at 0x7f1e48415990>
```




Episte
0.02
0.01
0.00
0
2500
5000
7500
10000
12500
15000
17500
Sample index


The aleatoric uncertainty
(probability entropy) of the predictions
Aleatoric uncertainty
1.2698
1.2696
1.2694
1.2692
1.2690
1.2688
1.2686
1.2684
0
2500
5000
7500
10000
12500
15000
17500
Sample index


The model misspecification uncertainty
(probability cross-entropy) of the predictions
Misspecification uncertainty
1.6
1.4
1.2
1.0
0.8
0
2500
5000
7500
10000
12500
15000
17500
Sample index


The complete measurement of prediction uncertainty
Prediction uncertainty
30
25
20
15
10
5
0
0
2500
5000
7500
10000
12500
15000
17500

Visualize the result of outlier detection on MNIST data set using BCNN

In [20]:

```
# Record the information about the index of outliers
location = (comp_uncer > threshold)
index = np.where(location)[0]
n_outliers = len(index)
print(np.mean(location)); print(n_outliers)

# Visualize the result of outlier detection on MNIST data set using BCNN
columns = 13; rows = int(n_outliers/columns) + 1 \
    if n_outliers%columns != 0 else int(n_outliers/columns)
figs, axes = plt.subplots(rows, columns, figsize = (columns, rows),
                          subplot_kw = {'xticks':[], 'yticks':[]},
                          gridspec_kw = dict(hspace = 0.4, wspace = 0.1))
plt.suptitle('Outlier detection on MNIST data set using BCNN',
             y = 0.9, fontsize = 15)
for i, ax in enumerate(axes.flat):
    if i < n_outliers:
        ax.imshow(features.numpy()[index[i]], cmap = 'binary', interpolation = 'nearest'
)
        ax.text(0.05, 0.05, str(int(mnist_data[['label']].values[index[i]])),
                transform = ax.transAxes, color = 'green')
        ax.set_xlabel('{:.2f}'.format(comp_uncer[index[i]]), color = 'red')
        ax.spines['top'].set_visible(False)
        ax.spines['right'].set_visible(False)
        ax.spines['bottom'].set_visible(False)
        ax.spines['left'].set_visible(False)
    else:
        ax.axis('off')
```

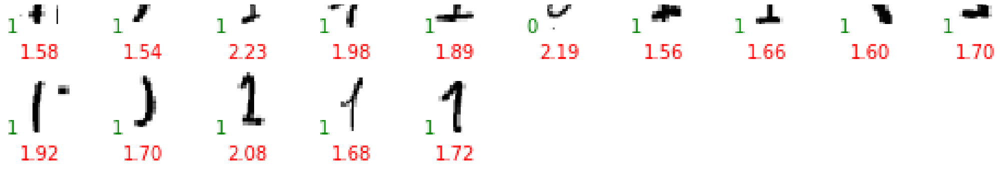
```
0.014293981481481482
247
```

Perform outlier detection on MNIST data set using LOF and DBSCAN method respectively, and visualize the results of these two methods

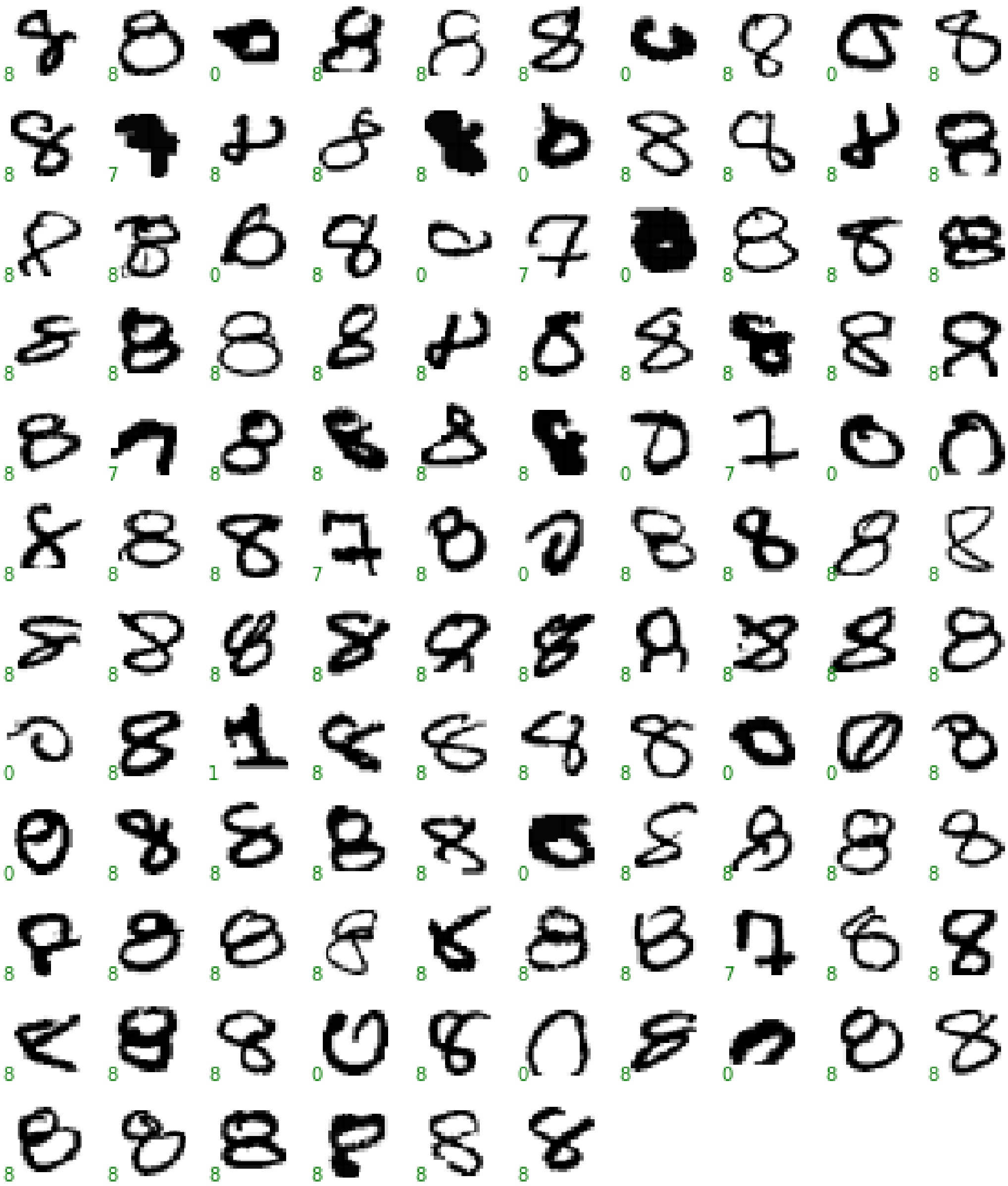
In [38]:

```
# Outlier detection on MNIST data set using Local Outlier Factor method
Lof = LocalOutlierFactor(); offset = -1.5
Lof.fit(mnist_data)
Lof_fac = Lof.negative_outlier_factor_
Lof_pre = (Lof_fac < offset).astype('int')
index_out = (Lof_pre == 1)
n_outliers = sum(index_out)
outliers_feature = mnist_data[index_out].drop('label', 1).\
                   values.reshape(n_outliers, 28, 28)
outliers_label = mnist_data[index_out]['label'].values

# Visualize the result of outlier detection on MNIST data set using LOF method
columns = 10; rows = int(n_outliers/columns) + 1 \
    if n_outliers%columns != 0 else int(n_outliers/columns)
figs, axes = plt.subplots(rows, columns, figsize = (columns, rows),
                          subplot_kw = {'xticks':[], 'yticks':[]},
                          gridspec_kw = dict(hspace = 0.4, wspace = 0.1))
plt.suptitle('Outlier detection on MNIST data set using LOF method', y = 0.9)
for i, ax in enumerate(axes.flat):
    if i < n_outliers:
        ax.imshow(outliers_feature[i], cmap = 'binary', interpolation = 'nearest')
        ax.text(0.05, 0.05, str(outliers_label[i]),
                transform = ax.transAxes, color = 'green')
        ax.set_xlabel('{:.2f}'.format(-Lof_fac[np.where(index_out)[0][i]]), color = 'red
')
        ax.spines['top'].set_visible(False)
        ax.spines['right'].set_visible(False)
        ax.spines['bottom'].set_visible(False)
        ax.spines['left'].set_visible(False)
    else:
        ax.axis('off')

# Outlier detection on MNIST data set using DBSCAN method
DBSCAN_model = DBSCAN(eps = 7.2, min_samples = 5)
```

```python
DBSCAN_fit = DBSCAN_model.fit(mnist_data)
DBSCAN_pre = DBSCAN_fit.labels_
index_noise = (DBSCAN_pre == -1); n_noise = sum(index_noise)
noise_feature = mnist_data[index_noise].drop('label', 1).\
                values.reshape(n_noise, 28, 28)
noise_label = mnist_data[index_noise]['label'].values

# Visualize the result of outlier detection on MNIST data set using DBSCAN method
columns = 10; rows = int(n_noise/columns) + 1 \
    if n_noise%columns != 0 else int(n_noise/columns)
figs, axes = plt.subplots(rows, columns, figsize = (columns, rows),
                          subplot_kw = {'xticks':[], 'yticks':[]},
                          gridspec_kw = dict(hspace = 0.1, wspace = 0.1))
plt.suptitle('Outlier detection on MNIST data set using DBSCAN method', y = 0.92)
for i, ax in enumerate(axes.flat):
    if i < n_noise:
        ax.imshow(noise_feature[i], cmap = 'binary', interpolation = 'nearest')
        ax.text(0.05, 0.05, str(noise_label[i]),
                transform = ax.transAxes, color = 'green')
        ax.spines['top'].set_visible(False)
        ax.spines['right'].set_visible(False)
        ax.spines['bottom'].set_visible(False)
        ax.spines['left'].set_visible(False)
    else:
        ax.axis('off')
```



Outlier detection on MNIST data set using DBSCAN method



Part 3 - The exploration on the Taxi data set

Load the Taxi data set
You first need to upload this data set to the following path on Kaggle: '../input/taxi-dataset/taxi.csv'

Perform some initial analyses on Taxi data set and remove the seasonal variation of Taxi data set

In [43]:

```
# Load the Taxi data set and use the 'timestamp' column as index
# You first need to upload this data set to the following path:
# '../input/taxi-dataset/taxi.csv'
taxi = pd.read_csv('../input/taxi-dataset/taxi.csv',
                   index_col = 'timestamp', parse_dates = True)
taxi.index.freq = '30T'

# Fix the random seed
set_seed(seed = 120)
```

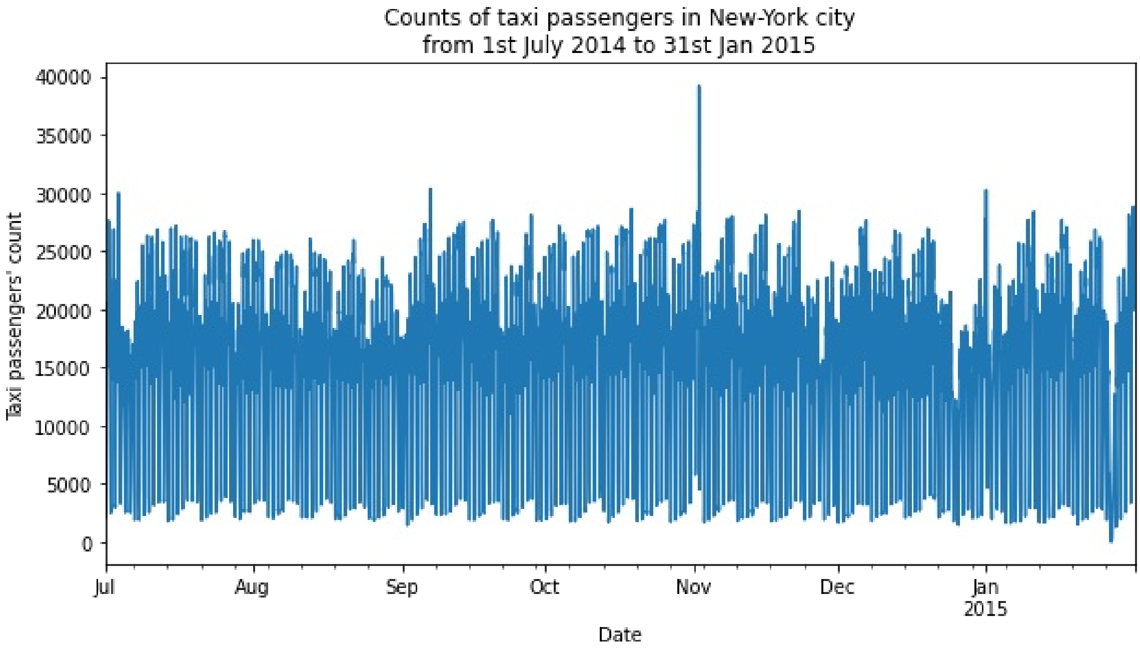
```
# Some initial analyses on Taxi data set
print(taxi.info()); display(taxi.describe())
taxi.plot(figsize = (10, 5), xlabel = 'Date', ylabel = 'Taxi passengers\' count',
          title = 'Counts of taxi passengers in New-York city\n' +
          'from 1st July 2014 to 31st Jan 2015').legend_.remove()

# Remove the seasonal variation of Taxi data set
period = 336
myfilter = np.hstack([1/(2*period), np.array([1/period for i in range(period - 1)]),
                      1/(2*period)])
taxi_decom = seasonal_decompose(taxi, filt = myfilter, period = period,
                                extrapolate_trend = 'freq')
taxi_DeSeason = taxi_decom.observed - taxi_decom.seasonal

# Visualize the Taxi data set after removing seasonal variation
plt.figure(figsize = (10, 5))
plt.plot(taxi_DeSeason.index, taxi_DeSeason.values)
plt.xlabel('Date'); plt.ylabel('Taxi passengers\' count')
plt.title('Counts of taxi passengers in New-York city after removing seasonal variation')
```

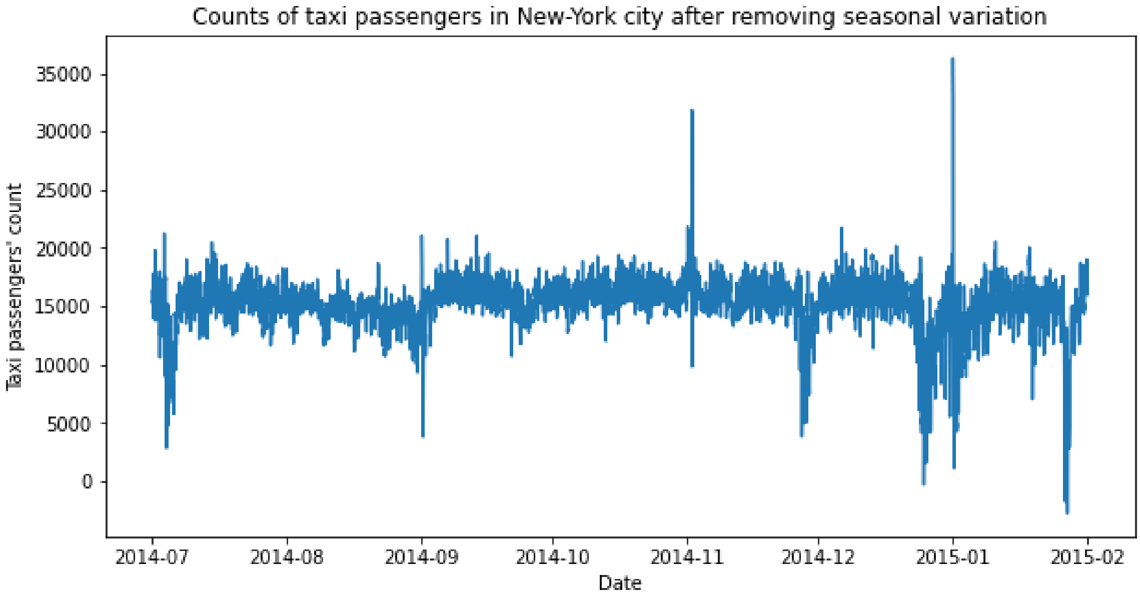
```
<class 'pandas.core.frame.DataFrame'>
DatetimeIndex: 10320 entries, 2014-07-01 00:00:00 to 2015-01-31 23:30:00
Freq: 30T
Data columns (total 1 columns):
 #   Column  Non-Null Count  Dtype
---  ------  --------------  -----
 0   value   10320 non-null  int64
dtypes: int64(1)
memory usage: 161.2 KB
None
```

	value
count	10320.000000
mean	15137.569380
std	6939.495808
min	8.000000
25%	10262.000000
50%	16778.000000
75%	19838.750000
max	39197.000000

Out[43]:

```
Text(0.5, 1.0, 'Counts of taxi passengers in New-York city after removing seasonal variat
ion')
```





Prepare the data used to train the model and split them into train, validation and test set

In [44]:

```
# Prepare the data used to train the model
# Prepare the features and target of Taxi data set separately, and
# convert the data set to "tensorflow.dataset" type
time = (taxi.index.values - np.datetime64('2014-07-01T00:00:00'))/np.timedelta64(1, '30m
')
taxi_data = np.vstack([time, taxi_DeSeason.values]).T
dataset_size = len(taxi_data) - 1
length = 24
features = np.zeros((dataset_size, length, 2))
for i in range(dataset_size):
    if i < length:
        features[i] = np.vstack([taxi_data[[0 for k in range(length - i - 1)]],
                                taxi_data[[k for k in range(i + 1)]]])
    else:
        features[i] = taxi_data[(i - length + 1):(i + 1)]
features = tf.constant(features)
labels = tf.constant(taxi_DeSeason.values[1:])
taxi_tfds = tf.data.Dataset.from_tensor_slices((features, labels)).\
    map(lambda x, y: (x, tf.cast(y, tf.float64))).\
    prefetch(buffer_size = dataset_size)

# Split the data set into train, validation and test set
train_size = round(dataset_size*0.8)
validation_size = round(dataset_size*0.1)
test_size = dataset_size - train_size - validation_size
taxi_tfds_veri = taxi_tfds.shuffle(buffer_size = dataset_size)
taxi_train = taxi_tfds_veri.take(train_size).batch(train_size)
taxi_validation = taxi_tfds_veri.skip(train_size).take(validation_size).batch(validation_
size)
taxi_test = taxi_tfds_veri.skip(train_size + validation_size).batch(test_size)
```

Construct and train the Bayesian LSTM neural network (BLSTMNN) model

In [ ]:

```
# Specify some model parameters
num_epochs = 5000
learning_rate = 0.5

# Define the loss function
# We still use the negative Evidence Lower Bound (-ELBO) as the loss function.
def negative_ELBO(label_true, label_pred):
    neg_log_likelihood = -tf.reduce_sum(label_pred.log_prob(label_true))
    kl = sum(taxi_model.losses)/train_size
```

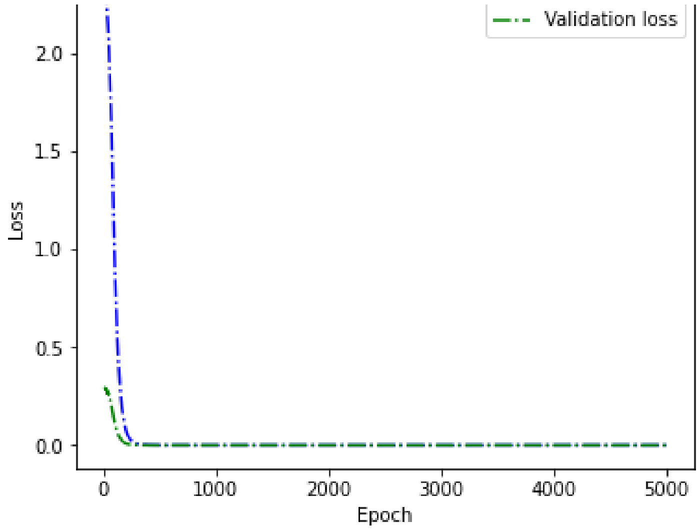
```
    return neg_log_likelihood + kl

# Construct the Bayesian LSTM neural network (BLSTMNN) model
BLSTM_layer1 = ed2.layers.LSTMCellFlipout(8, activation = 'sigmoid')
BLSTM_layer2 = ed2.layers.LSTMCellFlipout(16, activation = 'sigmoid')
taxi_model = tkeras.Sequential([
    tkeras.layers.Input(shape = (length, 2)),
    tkeras.layers.BatchNormalization(),
    tkeras.layers.RNN(cell = BLSTM_layer1, return_sequences = True),
    tkeras.layers.RNN(cell = BLSTM_layer2),
    tkeras.layers.Dense(units = 2),
    tfp.layers.IndependentNormal(1)
])

# View the structure of the model
taxi_model.summary()

# Compile the constructed Bayesian LSTM neural network
# I use the RMSprop optimizer with learning rate being equal to 0.5 to
# minimize the loss function, and use Mean Square Error (MSE) as the metric
# to evaluate the accuracy of the model.
taxi_model.compile(
    optimizer = tkeras.optimizers.RMSprop(learning_rate = learning_rate),
    loss = negative_ELBO,
    metrics = [tkeras.metrics.mean_squared_error]
)

# Fit the constructed Bayesian LSTM neural network with data
taxi_fit = taxi_model.fit(x = taxi_train, epochs = num_epochs,
                          validation_data = taxi_validation)
```

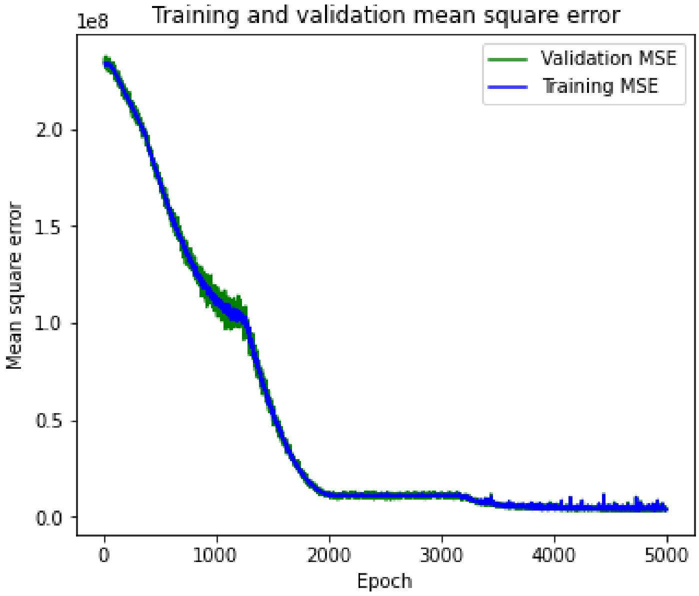
Draw the trend of the loss and the MSE on the train and validation set during the training process respectively

In [46]:

```
# Draw the trend of the loss and the MSE on the train and
# validation set during the training process respectively

# Prepare the data
train_loss = np.array(taxi_fit.history['loss'])
val_loss = np.array(taxi_fit.history['val_loss'])
train_eva = np.array(taxi_fit.history['mean_squared_error'])
val_eva = np.array(taxi_fit.history['val_mean_squared_error'])
inits = 10
epochs = np.array(range(inits, len(train_loss)))

# The trend of loss on the train and validation set
fig1 = plt.figure(figsize = (6, 5)); ax1 = plt.axes()
ax1.plot(epochs + 1, train_loss[epochs], 'b-.', label = 'Training loss')
ax1.plot(epochs + 1, val_loss[epochs], 'g-.', label = 'Validation loss')
ax1.set(xlabel = 'Epoch', ylabel = 'Loss',
        title = 'Training and validation loss')
ax1.legend()

# The trend of the metric (MSE) on the train and validation set
fig2 = plt.figure(figsize = (6, 5)); ax2 = plt.axes()
ax2.plot(epochs + 1, val_eva[epochs], 'g-', label = 'Validation MSE')
ax2.plot(epochs + 1, train_eva[epochs], 'b-', label = 'Training MSE')
ax2.set(xlabel = 'Epoch', ylabel = 'Mean square error',
        title = 'Training and validation mean square error')
ax2.legend()

# Evaluate the trained model on both train set and test set respectively
print(taxi_model.evaluate(taxi_train, verbose = 0))
print(taxi_model.evaluate(taxi_test, verbose = 0))
```

```
[70913.3203125, 3712179.25]
[9663.1689453125, 3677017.75]
```





I take 10 samples from the test set. Then, I construct and visualize the 95% confidence intervals for the predictions of these samples.

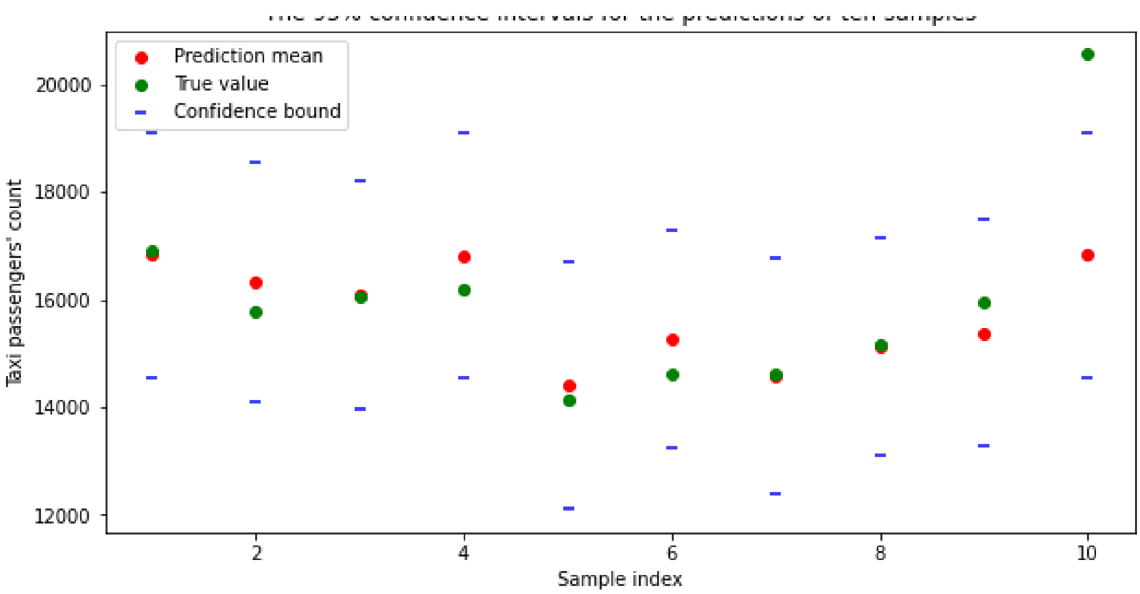
In [47]:

```
# Take 10 samples from the test set
num_exa = 10
features_exa, targets_exa = list(taxi_test.unbatch().batch(num_exa))[0]
features_exa = features_exa.numpy()
targets_exa = targets_exa.numpy()

# Compare the prediction means with the true labels
examples_mean = taxi_model(features_exa).mean().numpy()
examples_std = taxi_model(features_exa).stddev().numpy()

# Construct and visualize the 95% confidence intervals for the predictions
plt.figure(figsize = (10, 5))
index = range(1, num_exa + 1)
plt.scatter(index, examples_mean, color = 'red', label = 'Prediction mean')
plt.scatter(index, targets_exa, color = 'green', label = 'True value')
plt.scatter(index, examples_mean + 1.96*examples_std,
            color = 'blue', marker = '_', label = 'Confidence bound')
plt.scatter(index, examples_mean - 1.96*examples_std,
            color = 'blue', marker = '_')
plt.xlabel('Sample index'); plt.ylabel('Taxi passengers\' count')
plt.title('The 95% confidence intervals for the predictions of ten samples')
plt.legend()
```

Out[47]:

```
<matplotlib.legend.Legend at 0x7f2216bc8ed0>
```

The 95% confidence intervals for the predictions of ten samples



Clear the model and re-train the model with the whole data set

In [ ]:

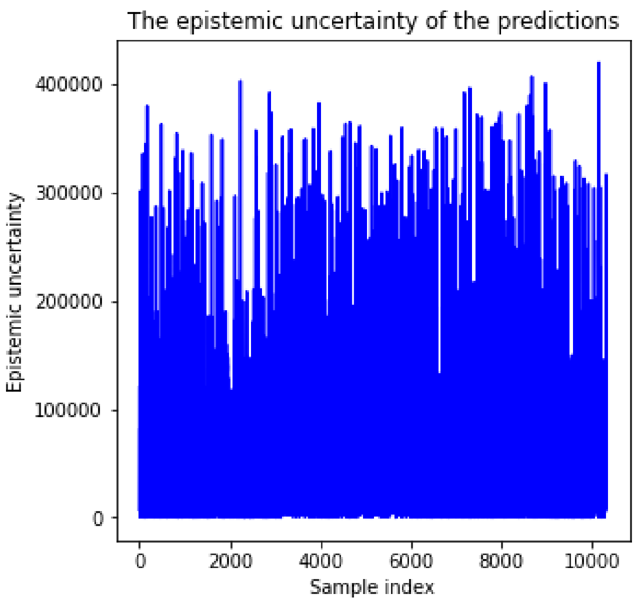
```
# Clear the model and re-train the model with the whole data set

# Re-define the loss function in order to update the weight for the
# KL divergence loss between the surrogate posterior and weight prior
def negative_ELBO(label_true, label_pred):
    neg_log_likelihood = -tf.reduce_sum(label_pred.log_prob(label_true))
    kl  = sum(taxi_model.losses)
    return neg_log_likelihood + kl/dataset_size

# Clear the model
BLSTM_layer1 = ed2.layers.LSTMCellFlipout(8, activation = 'sigmoid')
BLSTM_layer2 = ed2.layers.LSTMCellFlipout(16, activation = 'sigmoid')
taxi_model = tkeras.Sequential([
    tkeras.layers.Input(shape = (length, 2)),
    tkeras.layers.BatchNormalization(),
    tkeras.layers.RNN(cell = BLSTM_layer1, return_sequences = True),
    tkeras.layers.RNN(cell = BLSTM_layer2),
    tkeras.layers.Dense(units = 2),
    tfp.layers.IndependentNormal(1)
])

# Re-compile the model with the same settings
taxi_model.compile(
    optimizer = tkeras.optimizers.RMSprop(learning_rate = learning_rate),
    loss = negative_ELBO,
    metrics = [tkeras.metrics.mean_squared_error]
)

# Re-fit the model with the whole data set
taxi_model.fit(x = taxi_tfds.batch(dataset_size), epochs = num_epochs)
```

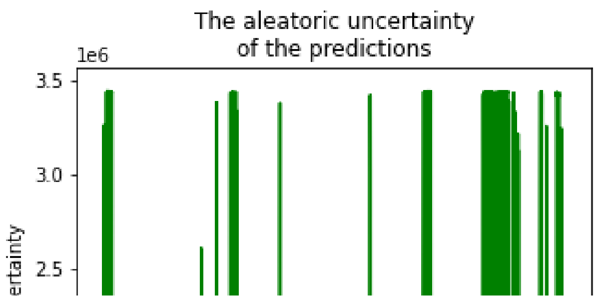
Quantify and plot all kinds of uncertainties of the predictions

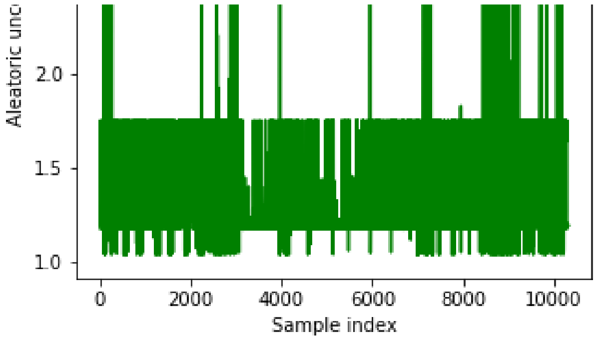
In [49]:

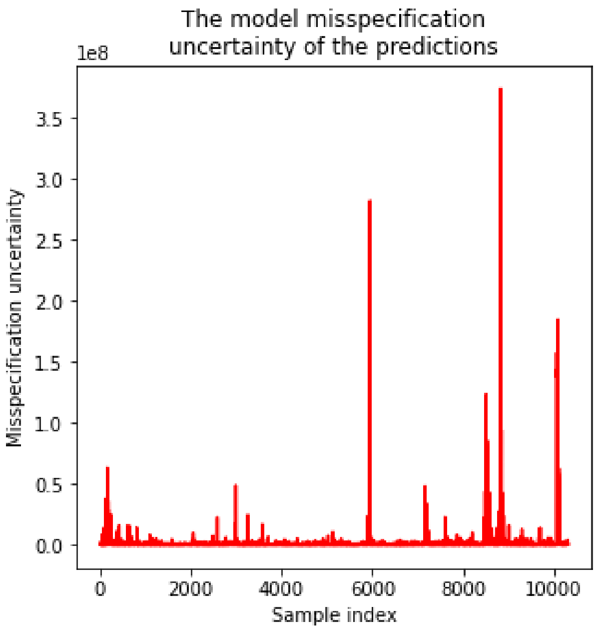
```
# Quantify all kinds of uncertainties of the predictions
N = 1000; records = np.zeros((N, dataset_size, 3))
for i in range(N):
    records[i, :, 0] = taxi_model(features).mean().numpy()[:, 0]
    records[i, :, 1] = taxi_model(features).variance().numpy()[:, 0]
    records[i, :, 2] = (taxi_model(features).mean().numpy()[:, 0] - labels.numpy())**2
epistemic = np.var(records[:, :, 0], axis = 0)
aleatoric = np.mean(records[:, :, 1], axis = 0)
misspecification = np.mean(records[:, :, 2], axis = 0)
P = 0; Q = 1/np.std(aleatoric); R = 6/np.std(misspecification)
W = -(Q*np.min(aleatoric) + R*np.min(misspecification))
```

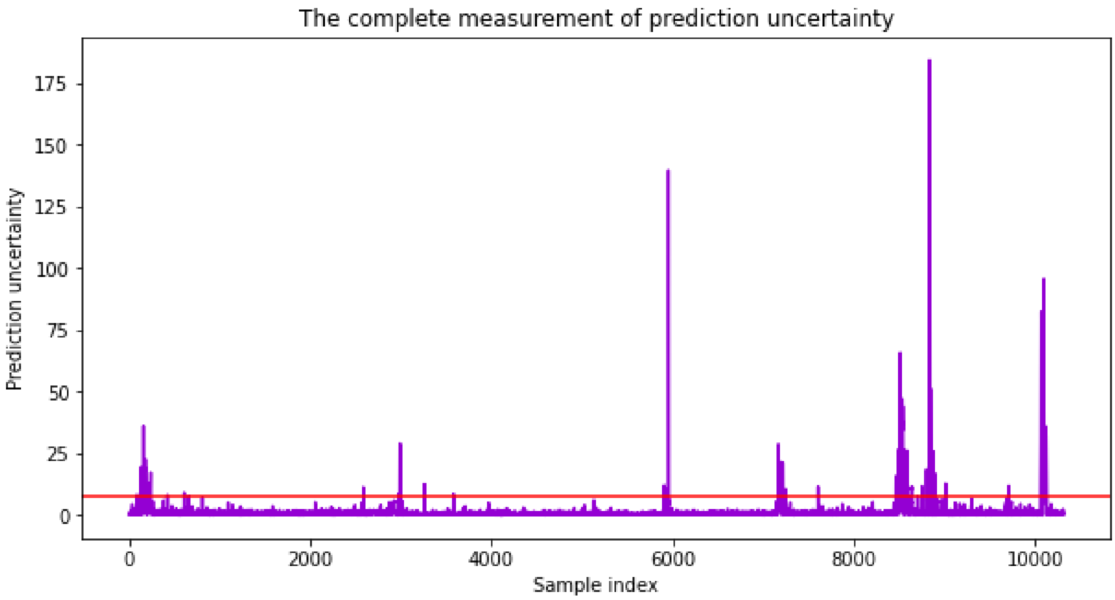
```
comp_uncer = P*epistemic + Q*aleatoric + R*misspecification + W

# Plot all kinds of uncertainties
X = range(1, dataset_size + 1)

# Plot the epistemic uncertainty
plt.figure(figsize = (5, 5))
plt.plot(X, epistemic, 'b-')
plt.xlabel('Sample index')
plt.ylabel('Epistemic uncertainty')
plt.title('The epistemic uncertainty of the predictions')

# Plot the aleatoric uncertainty
plt.figure(figsize = (5, 5))
plt.plot(X, aleatoric, 'g-')
plt.xlabel('Sample index')
plt.ylabel('Aleatoric uncertainty')
plt.title('The aleatoric uncertainty\nof the predictions')

# Plot the model misspecification uncertainty
plt.figure(figsize = (5, 5))
plt.plot(X, misspecification, 'r-')
plt.xlabel('Sample index')
plt.ylabel('Misspecification uncertainty')
plt.title('The model misspecification\nuncertainty of the predictions')

# Plot the total prediction uncertainty
plt.figure(figsize = (10, 5))
plt.plot(X, comp_uncer, color = 'darkviolet')
plt.xlabel('Sample index')
plt.ylabel('Prediction uncertainty')
plt.title('The complete measurement of prediction uncertainty')
threshold = np.quantile(comp_uncer, 0.975)
plt.axhline(threshold, color = 'red')

# Adjust the vectors that contain all kinds of uncertainties
# in order to facilitate performing outlier detection
epistemic = np.hstack([0, epistemic])
aleatoric = np.hstack([0, aleatoric])
misspecification = np.hstack([0, misspecification])
comp_uncer = np.hstack([0, comp_uncer])
```











Visualize the result of outlier detection on Taxi data set using BLSTMNN

In [53]:

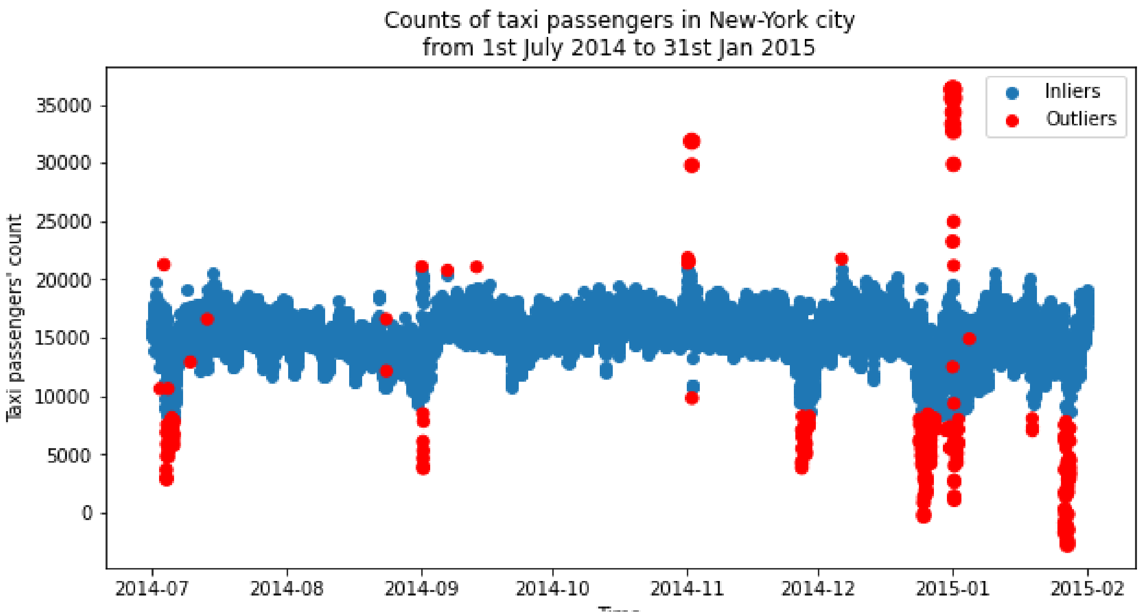
```
# Record the information about the index of outliers
threshold = np.quantile(comp_uncer, 0.975)
index = (comp_uncer > threshold)
n_outliers = np.sum(index)
print(np.mean(index)); print(n_outliers)

# Visualize the result of outlier detection on Taxi data set
# using Bayesian LSTM neural network
outliers = taxi_DeSeason[index]
inliers = taxi_DeSeason[(1 - index).astype('bool')]
fig = plt.figure(figsize = (10, 5)); ax = plt.axes()
ax.scatter(inliers.index, inliers.values, label = 'Inliers')
```

```
ax.scatter(outliers.index, outliers.values, color = 'red',
           s = plt.rcParams['lines.markersize']**2 + comp_uncer[index]/4)
ax.scatter([], [], color = 'red', label = 'Outliers')
ax.set(xlabel = 'Time', ylabel = 'Taxi passengers\' count',
       title = 'Counts of taxi passengers in New-York city\n' +
       'from 1st July 2014 to 31st Jan 2015')
plt.legend()

# Visualize the duration of the periods experiencing extremely high and extremely low
# taxi passenger numbers per day in New-York city respectively, and compare the dates
# of these extreme periods with the dates of special events happened in New York

# Prepare the data that we need
taxi_count = taxi.copy(); middle = 15000
taxi_count['value'] = taxi_DeSeason.values
large = []; small = []
for i in range(dataset_size + 1):
    x = 1 if (index[i] and taxi_DeSeason.values[i] > middle) else 0
    large.append(x)
    x = 1 if (index[i] and taxi_DeSeason.values[i] < middle) else 0
    small.append(x)
taxi_count['count_large'] = large
taxi_count['count_small'] = small
taxi_count = taxi_count.resample('D').sum().\
    apply(lambda x : 0.5*x).rename(columns = {'value' : 'busyness'})

# Visualize the duration of the extreme periods per day, and compare the
# dates of these extreme periods with the dates of special events in New-York
fig = plt.figure(figsize = (10, 5)); ax = plt.axes()
ax.plot(taxi_count.index, taxi_count['count_large'],
        color = 'red', label = 'Extremely high period')
ax.plot(taxi_count.index, taxi_count['count_small'],
        color = 'blue', label = 'Extremely low period')
events = ['Independence Day', 'School opening day', 'New-York marathon',
          'Thanksgiving Day', 'Christmas', 'New Year\'s Day', 'A snow storm']
dates = [pd.Timestamp('2014-7-4'), pd.Timestamp('2014-9-1'),
         pd.Timestamp('2014-11-2'), pd.Timestamp('2014-11-27'),
         pd.Timestamp('2014-12-25'), pd.Timestamp('2015-1-1'),
         pd.Timestamp('2015-1-26')]
colors = ['green', 'purple', 'yellow', 'brown', 'fuchsia', 'orange', 'cyan']
for event, date, color in zip(events, dates, colors):
    ax.axvline(date, label = event, color = color, linestyle = '--')
ax.set(xlabel = 'Date', ylabel = 'Period length (Hour)',
       title = 'Duration of extreme periods per day in New-York city')
plt.legend(bbox_to_anchor = (1.03, 0.5), loc = 6, borderaxespad = 0)
```

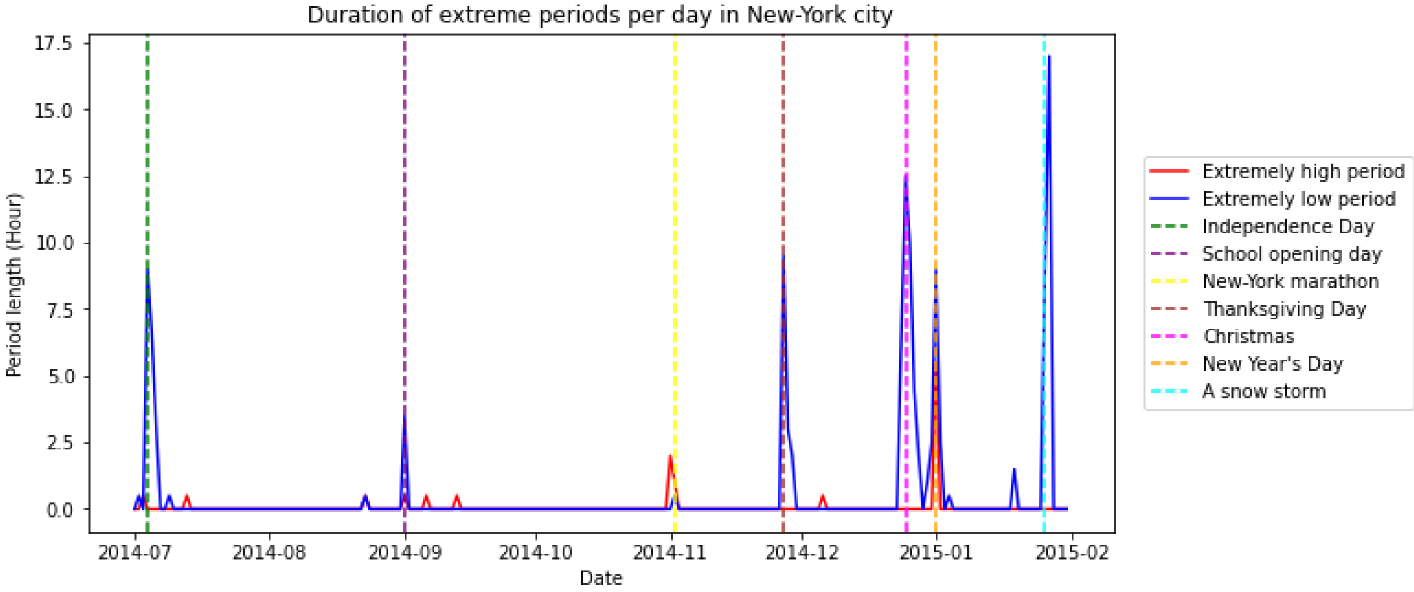
```
0.025
258
```

Out[53]:

```
<matplotlib.legend.Legend at 0x7f2214ea4a50>
```



Time



Perform outlier detection on Taxi data set using LOF and DBSCAN method respectively, and visualize the results of these two methods

In [54]:

```
# Prepare data for the LOF method and DBSCAN method
dataset_size = len(taxi_DeSeason)
taxi_detect = pd.DataFrame(
    np.array([range(dataset_size), taxi_DeSeason.values]).T,
    columns = ['time', 'counts']
)

# Outlier detection on Taxi data set using Local Outlier Factor method
Lof = LocalOutlierFactor(); offset_ = -1.45
Lof.fit(taxi_detect)
Lof_fac = Lof.negative_outlier_factor_
Lof_pre = -(Lof_fac < offset_).astype('int')
index_out = (Lof_pre == -1); index_in = (1 - index_out).astype('bool')
outliers = taxi_DeSeason[index_out]; inliers = taxi_DeSeason[index_in]

# Visualize the result of outlier detection on Taxi data set using LOF method
fig = plt.figure(figsize = (10, 5)); ax = plt.axes()
ax.scatter(inliers.index, inliers.values, c = Lof_pre[index_in],
           cmap = plt.cm.Dark2, label = 'Inliers')
ax.scatter(outliers.index, outliers.values, color = 'red',
           s = plt.rcParams['lines.markersize']**2 - 6*Lof_fac[index_out])
ax.scatter([], [], color = 'red', label = 'Outliers')
ax.set(xlabel = 'Time', ylabel = 'Taxi passengers\' count',
       title = 'Counts of taxi passengers in New-York city\n' +
       'from 1st July 2014 to 31st Jan 2015')
plt.legend()

# Outlier detection on Taxi data set using DBSCAN method
DBSCAN_model = DBSCAN(eps = 380, min_samples = 20)
DBSCAN_fit = DBSCAN_model.fit(taxi_detect)
DBSCAN_pre = DBSCAN_fit.labels_
index_noise = (DBSCAN_pre == -1); index_in = (1 - index_noise).astype('bool')
noise = taxi_DeSeason[index_noise]; inliers = taxi_DeSeason[index_in]

# Visualize the result of outlier detection on Taxi data set using DBSCAN method
fig = plt.figure(figsize = (10, 5)); ax = plt.axes()
ax.scatter(inliers.index, inliers.values, c = DBSCAN_pre[index_in],
           cmap = plt.cm.Dark2, label = 'Inliers')
ax.scatter(noise.index, noise.values, color = 'red', label = 'Outliers')
ax.set(xlabel = 'Time', ylabel = 'Taxi passengers\' count',
       title = 'Counts of taxi passengers in New-York city\n' +
       'from 1st July 2014 to 31st Jan 2015')
plt.legend()
```

Out[54]:

```
<matplotlib.legend.Legend at 0x7f1e1bb61d90>
```