Appendix

April 20, 2018

```
In [4]: import time
        import numpy as np
        import pandas as pd
        from scipy import stats
        pd.options.display.float_format = '{:,.3f}'.format

        # %matplotlib notebook
        import seaborn as sns
        sns.set(style="ticks", color_codes=True)
        import matplotlib.pyplot as plt

        from sklearn.decomposition import PCA, NMF
        from sklearn.manifold import TSNE
        from sklearn.model_selection import train_test_split
        from sklearn.metrics import mean_absolute_error

        from sklearn.neighbors import KNeighborsRegressor
        from sklearn.linear_model import LinearRegression, Ridge, Lasso, ElasticNet
        from sklearn.svm import SVR
        from sklearn.ensemble import BaggingRegressor, ExtraTreesRegressor
        from sklearn.tree import DecisionTreeRegressor
        from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
        from sklearn.neural_network import MLPRegressor

        class Data:
            #storage class for data
            def __init__(self, filename, subset_count=None):
                x = pd.read_csv(filename, index_col='id')
                if subset_count is not None: # Nice to use for testing
                    permut = np.random.permutation(x.shape[0])[:subset_count]
                    x = x.iloc[permut, :]

                self.df_y = x['loss']
                y = x['loss'].values
                del x['loss']

                convertedX = pd.get_dummies(x, drop_first=True)
```

```python
        X = convertedX.values
        self.X = X
        self.y = y

        self.df_X = convertedX
        self.df_X_test = None

    def get_split(self, test_size=0.20, pca_components=None, nmf_components=None):
        X_train, X_test, y_train, y_test = train_test_split(self.X, self.y,
                                                            test_size=test_size)
        if pca_components is not None:
            pca = PCA(n_components=pca_components)
            pca.fit(X_train)
            X_train = pca.transform(X_train)
            X_test = pca.transform(X_test)
        elif nmf_components:
            nmf = NMF(n_components=nmf_components)
            X_train = nmf.fit_transform(X_train)
            X_test = nmf.transform(X_test)
        return  X_train, X_test, y_train, y_test

    def remove_columns(self, columns):
        columns = tuple(columns)
        for col in self.df_X.columns:
            if col.startswith(columns):
                del self.df_X[col]
        self.X = self.df_X.values

    def read_test_data(self, filename):
        X_test = pd.read_csv(filename, index_col='id')
        X_test = pd.get_dummies(X_test, drop_first=True)

        additional_columns = set(X_test.columns) - set(self.df_X.columns)
        X_test = X_test.drop(columns=additional_columns)

        missing_columns = set(self.df_X.columns) - set(X_test.columns)
        for col in missing_columns:
            X_test[col] = 0

        self.df_X_test = X_test
        return X_test.values

def evaluate(name, estimator, X_train, X_test, y_train, y_test):
    t_0 = time.time()
    print(f'{name}:')
    estimator.fit(X_train, y_train)

    t_1 = time.time()
```

```
        print(f'\tTime elapsed for model construction {t_1 - t_0:.3f} sec')
        y_test_predict = estimator.predict(X_test)
        error_test = mean_absolute_error(y_test, y_test_predict)
        error_train = mean_absolute_error(y_train, estimator.predict(X_train))
        print(f'\tTime elapsed for prediction {time.time() - t_1:.3f} sec')
        print(f'\tTest error: {error_test:.3f}')
        print(f'\tTrain error: {error_train:.3f}')
        return error_test
```

```
In [ ]: # First overall test
        data = Data("train.csv")
        data.remove_columns(['cont9', 'cont12', 'cat2', 'cat3', 'cat4',
                             'cat5', 'cat6', 'cat7', 'cat8', 'cat86'])
        X_train, X_test, y_train, y_test = data.get_split()

        ESTIMATORS = {
            # Linear
            "LinearRegression": LinearRegression(n_jobs=-1),
            "Ridge": Ridge(),
            "Lasso": Lasso(),
            "ElasticNet": ElasticNet(),
            # Non-linear
            "BaggingRegressor": BaggingRegressor(n_jobs=-1),
            "ExtraTreesRegressor": ExtraTreesRegressor(n_jobs=-1),
            "RandomForestRegressor": RandomForestRegressor(n_jobs=-1),
            "GradientBoostingRegressor": GradientBoostingRegressor(loss='huber'),
            "MLP":  MLPRegressor(),
            "KNeighborsRegressor": KNeighborsRegressor(n_jobs=-1),
            "SVR": SVR(),
        }

        for name, estimator in ESTIMATORS.items():
            evaluate(name, estimator, X_train, X_test, y_train, y_test)
```

```
LinearRegression:
        Time elapsed for model construction 23.044 sec
        Time elapsed for prediction 0.478 sec
        Test error: 8798305800.629
        Train error: 1480.444
Ridge:
        Time elapsed for model construction 5.009 sec
        Time elapsed for prediction 0.391 sec
        Test error: 1477.830
        Train error: 1481.719
Lasso:
        Time elapsed for model construction 55.786 sec
        Time elapsed for prediction 0.389 sec
        Test error: 1481.435
```

```
        Train error: 1493.583
ElasticNet:
        Time elapsed for model construction 6.423 sec
        Time elapsed for prediction 0.389 sec
        Test error: 1745.976
        Train error: 1764.948
BaggingRegressor:
        Time elapsed for model construction 136.550 sec
        Time elapsed for prediction 34.328 sec
        Test error: 1519.984
        Train error: 605.857
ExtraTreesRegressor:
        Time elapsed for model construction 279.494 sec
        Time elapsed for prediction 1.537 sec
        Test error: 1535.685
        Train error: 0.072
RandomForestRegressor:
        Time elapsed for model construction 139.742 sec
        Time elapsed for prediction 1.370 sec
        Test error: 1519.550
        Train error: 602.167
GradientBoostingRegressor:
        Time elapsed for model construction 822.191 sec
        Time elapsed for prediction 1.641 sec
        Test error: 1444.904
        Train error: 1453.168
MLP:
        Time elapsed for model construction 2397.275 sec
        Time elapsed for prediction 2.283 sec
        Test error: 1410.916
        Train error: 1392.052
KNeighborsRegressor:
        Time elapsed for model construction 119.529 sec
        Time elapsed for prediction 17134.402 sec
        Test error: 1672.010
        Train error: 1364.940
SVR:
        Time elapsed for model construction 20007.080 sec
        Time elapsed for prediction 10160.075 sec
        Test error: 1755.613
        Train error: 1724.410
```

```
In [ ]: ESTIMATORS = {
            # Linear
            "LinearRegression": LinearRegression(n_jobs=-1),
            "Ridge": Ridge(),
            "Lasso": Lasso(),
```

```python
            "ElasticNet": ElasticNet(),
            # Non-linear
            "BaggingRegressor": BaggingRegressor(n_jobs=-1),
            "ExtraTreesRegressor": ExtraTreesRegressor(n_jobs=-1),
            "RandomForestRegressor": RandomForestRegressor(n_jobs=-1),
            "GradientBoostingRegressor": GradientBoostingRegressor(loss='huber'),
            "MLP":  MLPRegressor(),
        }

        # Test PCA and NMF
        data = Data("train.csv")

        X_train, X_test, y_train, y_test = data.get_split(pca_components=120)
        print(f'PCA with 120 components')
        for name, estimator in ESTIMATORS.items():
            evaluate(name, estimator, X_train, X_test, y_train, y_test)

        X_train, X_test, y_train, y_test = data.get_split(nmf_components=90)
        print(f'NMF with 90 components')
        for name, estimator in ESTIMATORS.items():
            evaluate(name, estimator, X_train, X_test, y_train, y_test)
```

```
PCA with 120 components
LinearRegression:
        Time elapsed for model construction 1.222 sec
        Time elapsed for prediction 0.052 sec
        Test error: 1336.491
        Train error: 1326.450
Ridge:
        Time elapsed for model construction 0.375 sec
        Time elapsed for prediction 0.047 sec
        Test error: 1336.488
        Train error: 1326.447
Lasso:
        Time elapsed for model construction 0.735 sec
        Time elapsed for prediction 0.050 sec
        Test error: 1335.520
        Train error: 1325.040
ElasticNet:
        Time elapsed for model construction 0.688 sec
        Time elapsed for prediction 0.059 sec
        Test error: 1503.928
        Train error: 1487.781
BaggingRegressor:
        Time elapsed for model construction 159.103 sec
        Time elapsed for prediction 7.503 sec
        Test error: 1385.234
        Train error: 551.043
```

```
ExtraTreesRegressor:
        Time elapsed for model construction 37.692 sec
        Time elapsed for prediction 0.782 sec
        Test error: 1379.454
        Train error: 0.001
RandomForestRegressor:
        Time elapsed for model construction 151.161 sec
        Time elapsed for prediction 0.754 sec
        Test error: 1390.771
        Train error: 552.164
GradientBoostingRegressor:
        Time elapsed for model construction 333.502 sec
        Time elapsed for prediction 0.793 sec
        Test error: 1317.153
        Train error: 1290.940
MLP:
        Time elapsed for model construction 327.754 sec
        Time elapsed for prediction 1.168 sec
        Test error: 1224.814
        Train error: 1195.139

NMF with 90 components
LinearRegression:
        Time elapsed for model construction 0.858 sec
        Time elapsed for prediction 0.047 sec
        Test error: 1372.249
        Train error: 1369.867
Ridge:
        Time elapsed for model construction 0.288 sec
        Time elapsed for prediction 0.031 sec
        Test error: 1367.990
        Train error: 1366.349
Lasso:
        Time elapsed for model construction 1.047 sec
        Time elapsed for prediction 0.047 sec
        Test error: 1380.740
        Train error: 1380.795
ElasticNet:
        Time elapsed for model construction 0.509 sec
        Time elapsed for prediction 0.047 sec
        Test error: 1969.046
        Train error: 1961.323
BaggingRegressor:
        Time elapsed for model construction 63.872 sec
        Time elapsed for prediction 6.347 sec
        Test error: 1350.245
        Train error: 536.754
ExtraTreesRegressor:
```

```
        Time elapsed for model construction 28.637 sec
        Time elapsed for prediction 0.648 sec
        Test error: 1359.542
        Train error: 0.009
RandomForestRegressor:
        Time elapsed for model construction 59.382 sec
        Time elapsed for prediction 0.608 sec
        Test error: 1344.332
        Train error: 537.979
GradientBoostingRegressor:
        Time elapsed for model construction 150.457 sec
        Time elapsed for prediction 0.901 sec
        Test error: 1263.213
        Train error: 1253.464
MLP:
        Time elapsed for model construction 1372.075 sec
        Time elapsed for prediction 6.929 sec
        Test error: 1363.668
        Train error: 1361.900
```

```
In [ ]: data = Data("train.csv")
        X_train, X_test, y_train, y_test = data.get_split()
        for n_estimators in np.arange(200, 601, 50):
            estimator = GradientBoostingRegressor(loss='huber', alpha=0.5,
                                                  n_estimators=n_estimators, max_depth=6,
                                                  learning_rate=0.1, min_samples_leaf=10,
                                                  min_samples_split=10)
            evaluate(f'GBR n_estimators={n_estimators}',
                     estimator, X_train, X_test, y_train, y_test)
```

```
GBR n_estimators=200:
        Time elapsed for model construction 9316.946 sec
        Time elapsed for prediction 4.889 sec
        Test error: 1163.757
        Train error: 1086.791
GBR n_estimators=250:
        Time elapsed for model construction 5754.714 sec
        Time elapsed for prediction 4.712 sec
        Test error: 1162.030
        Train error: 1076.098
GBR n_estimators=300:
        Time elapsed for model construction 6771.478 sec
        Time elapsed for prediction 5.666 sec
        Test error: 1160.265
        Train error: 1066.413
GBR n_estimators=350:
        Time elapsed for model construction 23563.061 sec
```

```
        Time elapsed for prediction 7.427 sec
        Test error: 1159.374
        Train error: 1057.450
GBR n_estimators=400:
        Time elapsed for model construction 8711.057 sec
        Time elapsed for prediction 7.002 sec
        Test error: 1158.555
        Train error: 1052.084
GBR n_estimators=450:
        Time elapsed for model construction 9692.810 sec
        Time elapsed for prediction 7.645 sec
        Test error: 1158.072
        Train error: 1046.006
GBR n_estimators=500:
        Time elapsed for model construction 10792.895 sec
        Time elapsed for prediction 8.363 sec
        Test error: 1158.072
        Train error: 1039.049
GBR n_estimators=550:
        Time elapsed for model construction 12230.542 sec
        Time elapsed for prediction 10.199 sec
        Test error: 1152.069
        Train error: 1031.342
GBR n_estimators=600:
        Time elapsed for model construction 14028.412 sec
        Time elapsed for prediction 14.199 sec
        Test error: 1142.065
        Train error: 1025.139
```

In [17]:
```
# Reading in the final test data
data = Data("train.csv")
X_train, y_train = data.df_X, data.df_y
X_test = data.read_test_data("test.csv")
X_test = data.df_X_test

estimator = GradientBoostingRegressor(loss='huber', alpha=0.5,
                                      n_estimators=600, max_depth=6,
                                      learning_rate=0.1, min_samples_leaf=10,
                                      min_samples_split=10)

t_0 = time.time()
estimator.fit(X_train, y_train)

t_1 = time.time()
print(f'Time elapsed for model construction {t_1 - t_0:.3f} sec')

y_test_predict = estimator.predict(X_test)
```

```
X_test['loss'] = y_test_predict
X_test['loss'].to_csv("GBR-submission.csv", header=True)
```

```
Time elapsed for model construction 10289.486 sec
```

```
In [21]: data = Data("train.csv")
         X_train, y_train = data.df_X, data.df_y
         X_test = data.read_test_data("test.csv")
         X_test = data.df_X_test

         nmf = NMF(n_components=90)
         X_train_trans = nmf.fit_transform(X_train)
         X_test_trans = nmf.transform(X_test)

         gbr = GradientBoostingRegressor(loss='huber', alpha=0.5,
                                         n_estimators=600, max_depth=6,
                                         learning_rate=0.1, min_samples_leaf=10,
                                         min_samples_split=10)

         t_0 = time.time()
         gbr.fit(X_train_trans, y_train)

         t_1 = time.time()
         print(f'Time elapsed for model construction {t_1 - t_0:.3f} sec')

         y_test_predict = gbr.predict(X_test_trans)

         X_test['loss'] = y_test_predict
         X_test['loss'].to_csv("GBR-NMF-submission.csv", header=True)
```

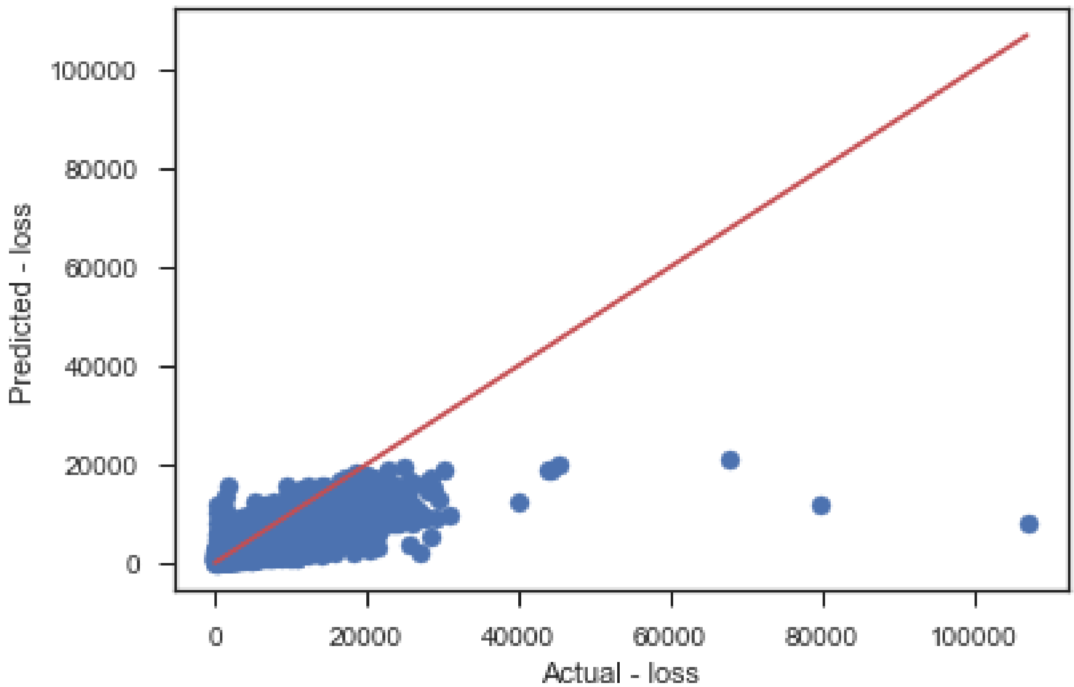
```
Time elapsed for model construction 3228.545 sec
```

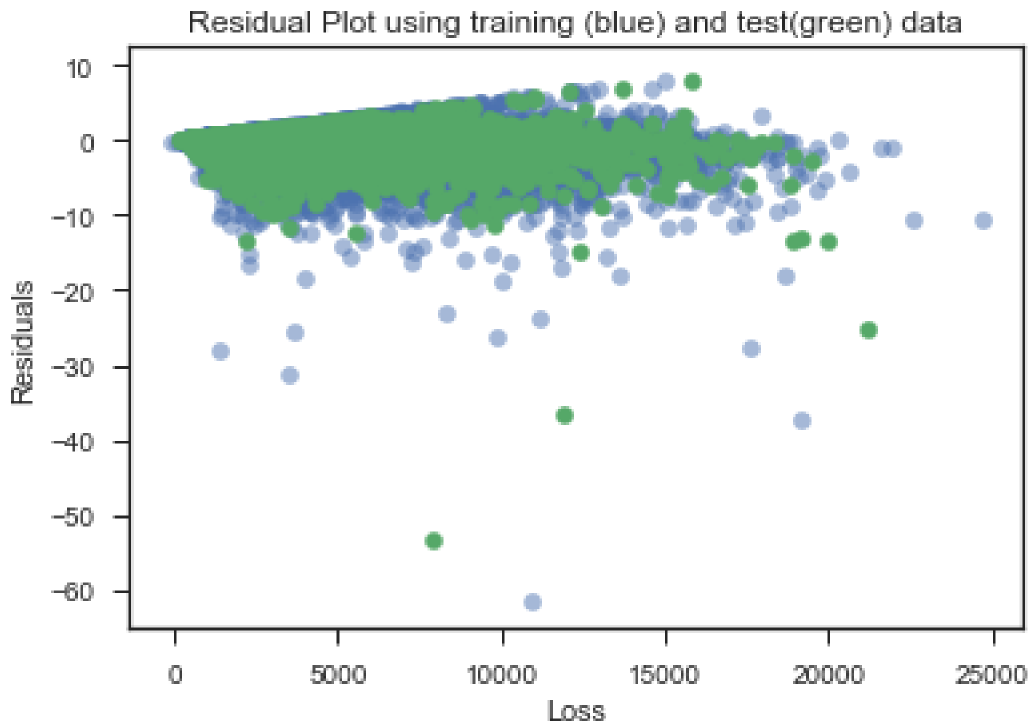
```
In [24]: X_train, X_test, y_train, y_test = data.get_split()
         X_train = nmf.transform(X_train)
         X_test = nmf.transform(X_test)

         y_test_predict = gbr.predict(X_test)
         y_train_predict = gbr.predict(X_train)

         # Plot of predicted values versus the true values
         plt.figure()
         plt.scatter(y_test, y_test_predict)
         plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r')
         plt.ylabel('Predicted - loss')
         plt.xlabel('Actual - loss')
```

```python
# Plot of residuals
plt.figure()
plt.scatter(y_train_predict, stats.zscore(y_train_predict - y_train),
                                                      c='b', s=40, alpha=0.5)
plt.scatter(y_test_predict, stats.zscore(y_test_predict - y_test),
                                                      c='g', s=40)
plt.hlines(y=0, xmin=0, xmax=20)
plt.title('Residual Plot using training (blue) and test(green) data')
plt.ylabel('Residuals')
plt.xlabel('Loss')
plt.show()
```






```
In [20]: data = Data("train.csv")
         X_train, y_train = data.df_X, data.df_y
         X_test = data.read_test_data("test.csv")
         X_test = data.df_X_test

         nmf = NMF(n_components=90)
         X_train_trans = nmf.fit_transform(X_train)
         X_test_trans = nmf.transform(X_test)

         y_train_trans = np.log1p(y_train)

         gbr = GradientBoostingRegressor(loss='huber', alpha=0.5,
                                         n_estimators=600, max_depth=6,
                                         learning_rate=0.1, min_samples_leaf=10,
                                         min_samples_split=10)

         t_0 = time.time()
         gbr.fit(X_train_trans, y_train_trans)

         t_1 = time.time()
         print(f'Time elapsed for model construction {t_1 - t_0:.3f} sec')

         y_test_predict = np.expm1(gbr.predict(X_test_trans))
```

```python
X_test['loss'] = y_test_predict
X_test['loss'].to_csv("GBR-NMF-log-submission.csv", header=True)
```

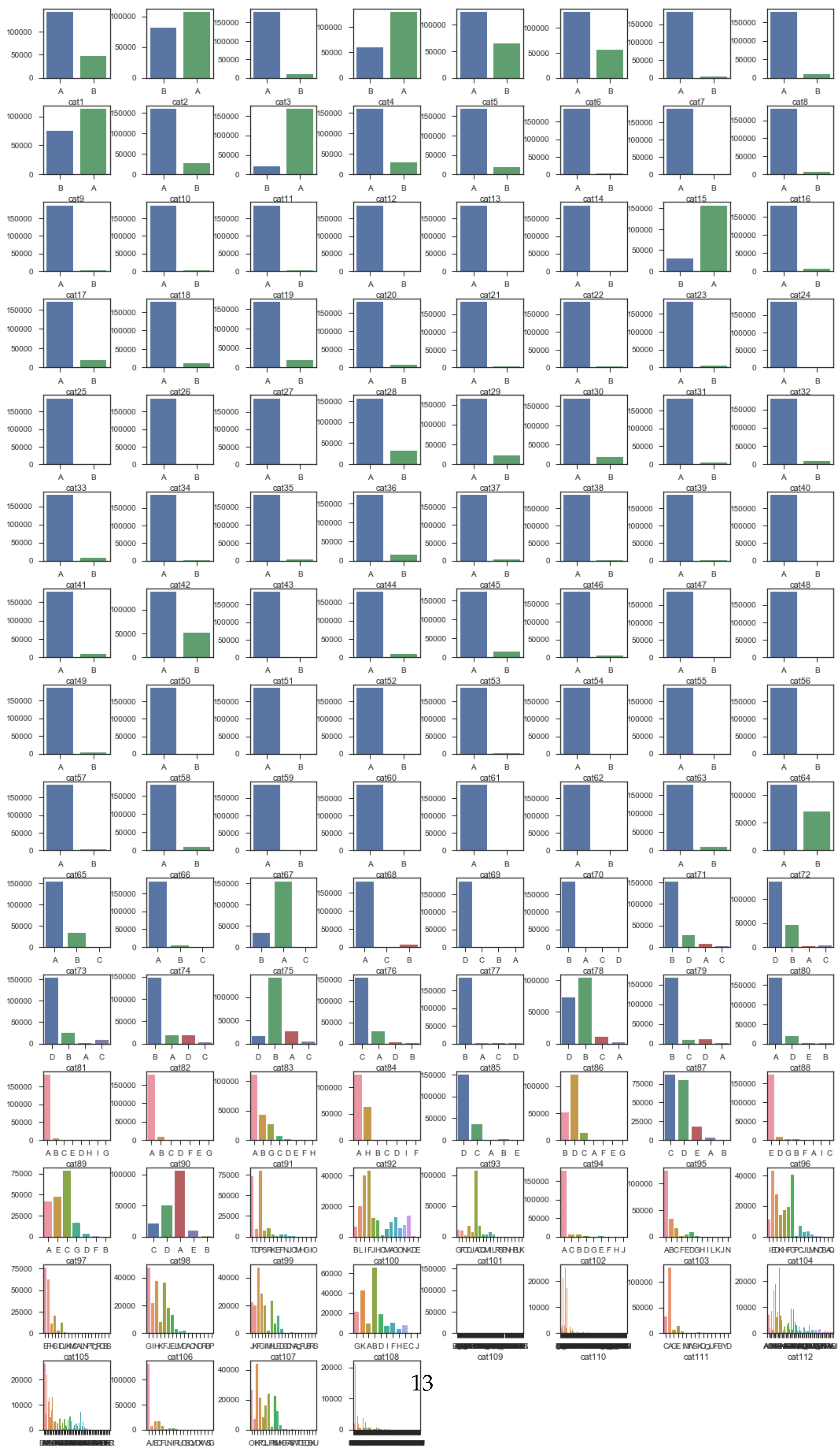
```
Time elapsed for model construction 2696.148 sec
```

In [6]:
```python
X_train = pd.read_csv("train.csv", index_col='id')

# Count the number of items for each categorical attribute
cat_index = [x for x in X_train.columns if x.startswith('cat')]

n = 8
r = len(cat_index)//n + 1
plt.figure(figsize=(18, 30))
for i in range(r):
    for j in range(n if i != r-1
                     else ((len(cat_index)%n))
                  ):
        if (i*n + j + 1) > len(cat_index):
            break
        plot = plt.subplot(r, n, (i*n + j + 1))
        ax = sns.countplot(x=cat_index[i*n + j], data=X_train)
        plt.subplots_adjust(wspace=0.55, hspace=0.4, top=0.96)
        ax.set_ylabel('')
plt.suptitle('The counts for each categorical attribute')
plt.show()
```

The counts for each categorical attribute



In [8]:
```
cat_index = [x for x in X_train.columns if x.startswith('cat')]

def letter_to_numb(series):
    ret = []
    for c in series:
        if len(c) == 1:
            ret.append(ord(c.lower()) - 96)
        else:
            ret.append('')
            for s in c:
                ret[-1] += str(ord(s.lower()) - 96)
            ret[-1] = int(ret[-1])
    return ret


integer_categories = X_train[cat_index].apply(letter_to_numb)

# spearman and kendall-tau mostly agree
corr = integer_categories.corr(method='kendall')

corr_matrix = corr.abs()
sorted_corr = (corr_matrix.where(np.triu(np.ones(corr_matrix.shape),
                                         k=1).astype(np.bool))
                 .stack()
                 .sort_values(ascending=False))
print('The most correlated categorical attributes are:')
sorted_corr[sorted_corr > 0.87]
```

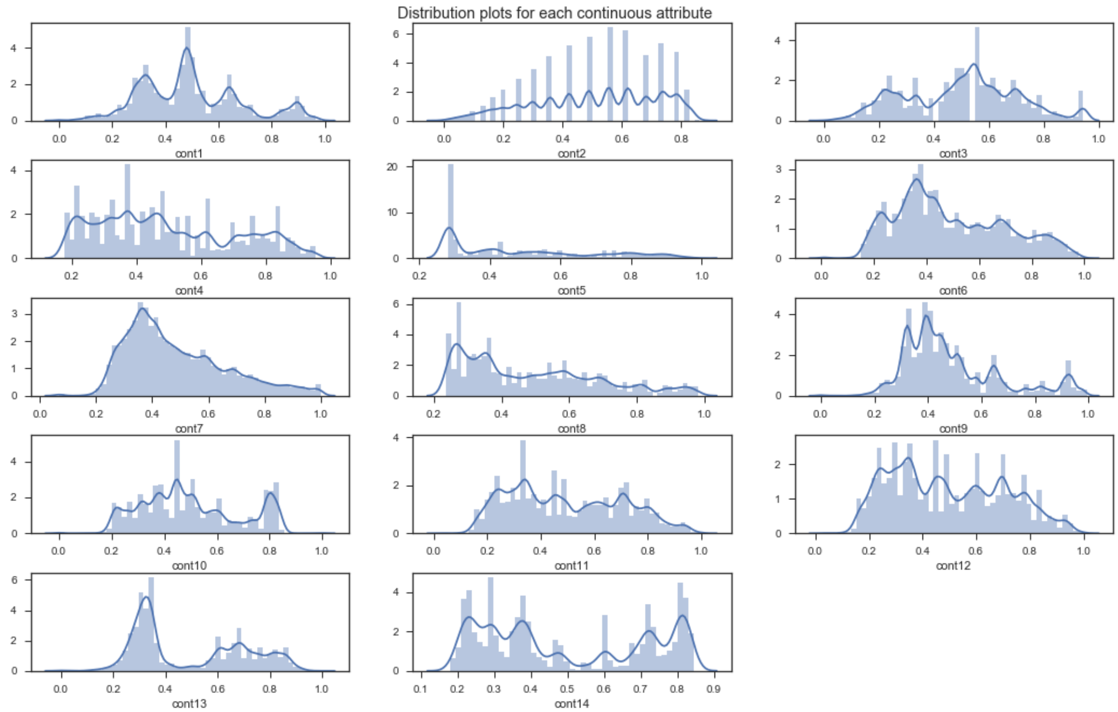
```
The most correlated categorical attributes are:
```

Out[8]:
```
cat7   cat89    0.999
cat3   cat90    0.998
cat8   cat102   0.991
cat4   cat111   0.934
cat2   cat9     0.932
cat6   cat50    0.926
       cat114   0.925
cat5   cat103   0.925
cat86  cat99    0.888
dtype: float64
```

In [9]:
```
cont_index = lambda : [x for x in X_train.columns if x.startswith('cont')]
plt.figure(figsize=(18, 10))

n = len(cont_index())
```

```
    for i, col in enumerate(cont_index()):
        plot = plt.subplot(n//3+1, 3, i + 1)
        sns.distplot(X_train[col])
        plot.set_xlabel(f'{col}')
        plt.subplots_adjust(hspace=0.4, top=0.96)
    plt.suptitle('Distribution plots for each continuous attribute')
    plt.show()
```




```
In [ ]: #Keras code
        import tensorflow, time
        import os
        import numpy
        from keras.models import Sequential
        from keras.layers import Dense, Activation, BatchNormalization
        from keras.layers import Dropout
        import keras.callbacks
        from keras import optimizers
        from keras import regularizers
        from keras.constraints import maxnorm
        from sklearn.decomposition import PCA
        from sklearn.feature_selection import VarianceThreshold, SelectKBest, f_regression
        from sklearn.model_selection import train_test_split

        def TestEstimator(name, estimator, X_train, y_train, X_test, y_test, tf = False):
```

```
    t=time.time()
    if tf:
        y_train_ = numpy.log1p(y_train)
    else:
        y_train_ = y_train

    estimator.fit(X_train, y_train_)
    trainTime = time.time()-t
    t = time.time()

    y_pred = estimator.predict(X_test)
    if tf:
        y_pred = numpy.expm1(y_pred)
    predictTime = time.time()-t

    y_train_pred = estimator.predict(X_train)
    if tf:
        y_train_pred = numpy.expm1(y_train_pred)

    error = numpy.sum(numpy.abs(y_pred - y_test)) / len(y_test)
    error_train = numpy.sum(numpy.abs(y_train_pred - y_train)) / len(y_train)
    #print(time.ctime(),name,error,trainTime,predictTime)
    return error_train, error #a difference here indicates divergence

EPOCHS = 100
class CustomMLPRegressor:
    """provide a similar interface to the sklearn regressors"""
    def LoadFromFile(self, filename):
        self.model = keras.models.load_model(filename)

    def __init__(self, nodes, earlyStopping, dropout):

        if type(nodes) is int:
            nodes = (nodes,)
        self.nodes = nodes
        self.dropout = dropout
        self.earlyStopping = earlyStopping

    def fit(self, X, y):
        #print (X,y)
        inputDim = X.shape[1]
        model = Sequential()
        self.model = model
        for i, nodeCount in enumerate(self.nodes):
            if i == 0:
                if len(self.nodes) == 1:
                    self.model.add(Dense(nodeCount,
                                         input_dim = inputDim,
```

```
                                          activation='relu'))
                    else:
                        self.model.add(Dense(nodeCount,
                                          input_dim = inputDim,
                                          ctivation='relu',
                                          kernel_constraint = maxnorm(3)))
                        if self.dropout:
                            model.add(Dropout(self.dropout))
                else:
                    if len(self.nodes) > i+1:
                        self.model.add(Dense(nodeCount,
                                          activation='relu',
                                          kernel_constraint = maxnorm(3)))
                        if self.dropout:
                            model.add(Dropout(self.dropout))
                    else:
                        self.model.add(Dense(nodeCount,  activation='relu'))
            model.add(Dense(1))
            opt = optimizers.Nadam()
            model.compile(loss='mae', optimizer=opt)
            #self.model = model

            callback_list = []
            filepath="weights-best.hdf5"
            checkpoint = keras.callbacks.ModelCheckpoint(filepath,
                                                        monitor='val_loss',
                                                        verbose=0, save_best_only=True,
                                                        mode='min')
            callback_list.append(checkpoint)
            earlyStopper = keras.callbacks.EarlyStopping(min_delta= self.earlyStopping,
                                                   patience=5,verbose=0)
            callback_list.append(earlyStopper

            history=model.fit(X.values.astype('float32'), y.astype('float32'),
                  epochs=EPOCHS, batch_size=1000,
                  verbose=2,validation_split=0.2,callbacks=callback_list)
            bestModel = keras.models.load_model('weights-best.hdf5')
            self.history = history
            self.model =bestModel
            return self
        def predict(self, X):
            #print ('predicting')
            ret =  self.model.predict(X.astype('float32'))
            #print (ret.shape)
            return ret.flatten()
    def TestMLP(mlp):
        e_train, e_test = TestEstimator('mlp',mlp, X_train, y_train,
                                     X_test, y_test, tf=False)
```

```
    print("mlp-%s-%.2f: %.2f %.2f"%(mlp.nodes,mlp.dropout,e_train, e_test))
    try:
        os.rename('weights-best.hdf5',
                  'weights-best-%.2f-%.2f-%s.hdf5'%(e_test,mlp.dropout,mlp.nodes))
    except FileExistsError:
        pass
    return e_train, e_test
#the following code was used to populate a results list.
# The lowest result for nodes/dropout pair was used to represent that
# point on the dataplot.
for i in range(2):
    nodes = 425+i*75
    for j in range(3):
        dropout =0.2+j*0.05
        mlp = CustomMLPRegressor((nodes,50,10),0.0,dropout)
        e_train, e = TestMLP(mlp)
        results.append([nodes,dropout,e_train, e])
        if e < bestE:
            bestE = e
            bestMLP = mlp
```