# HDS5230 Final Exam - programming - Miao Cai

May 12, 2019

## 1 HDS 5230 High Performance Computing

## 1.1 Final Exam - Progamming Part

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#### 2 Introduction

The big goal of this project is to use the provided dataset on health insurance charges to create a model that predicts charges as accurately as possible, based on the patient traits of age, sex, bmi, children, smoker, and region. As I generate this model, I performed and documented initial data quality checks, exploratory data analysis, and all of the models I tried to fit.

## 3 Methods summary

All the data cleaning, visualization, and modeling were conducted in Python, and this reported was wrote in jupyternotebook. The Python session and package version information is shown below.

```
In [38]: import os
    import sys
    import pathlib
    from tableone import TableOne
    import pandas as pd
    import numpy as np
    import seaborn as sns
    import h2o
    from h2o.estimators.glm import H2OGeneralizedLinearEstimator

    print(sys.version)
    print("Pandas version: {0}".format(pd.__version__))
    print("Numpy version:{0}".format(np.__version__))
    print("Seaborn version:{0}".format(sns.__version__))
    print("h2o version:{0}".format(h2o.__version__))
    print("My working directory:\n" + os.getcwd())
```

```
3.7.1 (default, Dec 14 2018, 13:28:58)
[Clang 4.0.1 (tags/RELEASE_401/final)]
```

Pandas version: 0.23.4 Numpy version: 1.15.4 Seaborn version:0.9.0 h2o version:3.22.1.3 My working directory:

/Users/miaocai/Dropbox/@2018 SPRING HDS5230 High performance computing/HDS5230Homework/Final es

#### 3.0.1 Loss function

I pick the loss function as the mean absolute error (MAE). I chose this loss function since the outcome variable charges are highly right-skewed. Using the most commonly used mean square error (MSE) will not be as robust as MAE since the error will be squared, which is strongly influenced by outliers.

#### 3.0.2 Initiate h2o and read data

```
In [39]: h2o.init(ip='localhost', port=54321, nthreads=-1, max_mem_size='2G')
```

Checking whether there is an H2O instance running at http://localhost:54321. connected.

Warning: Your H2O cluster version is too old (3 months and 17 days)! Please download and insta

18 hours 33 mins H20 cluster uptime: H2O cluster timezone: America/Chicago

H2O data parsing timezone: UTC H2O cluster version: 3.22.1.3

H2O cluster version age: 3 months and 17 days !!!

H2O cluster name: H20\_from\_python\_miaocai\_k7904q

H2O cluster total nodes:

H2O cluster free memory: 1.963 Gb

H2O cluster total cores: H2O cluster allowed cores: 8

H2O cluster status: locked, healthy

http://localhost:54321 H2O connection url:

H2O connection proxy:

H2O internal security: False

H20 API Extensions: XGBoost, Algos, AutoML, Core V3, Core V4

Python version: 3.7.1 final

```
In [40]: d0 = h2o.import_file("insurance.csv")
```

Parse progress: || 100%

After reading the .csv file by using h2o, I found that there are no missing values in the data, which is great!

#### 3.0.3 Split into train/validation/testing splits

We then need to convert some categorical variables into factors, and split the data into train, test, and validation sets.

#### 4 Results

#### 4.1 Summary statistics of model input variables

```
In [43]: d = pd.read_csv("insurance.csv")
         col_types = d.dtypes.to_dict()
         col_types['age'] = 'float64'
         d = pd.read_csv("insurance.csv", dtype=col_types)
         overall_table = TableOne(
             d, columns = ['age', 'bmi', 'children', 'smoker', 'region'],
             categorical = ['children', 'smoker', 'region'],
             groupby = 'sex', label_suffix=True, pval = True)
         overall_table
Out [43]:
                                   Grouped by sex
                                           isnull
                                                        female
                                                                        male
                                                                              pval
         variable
                         level
                                                            662
                                                                         676
         n
```

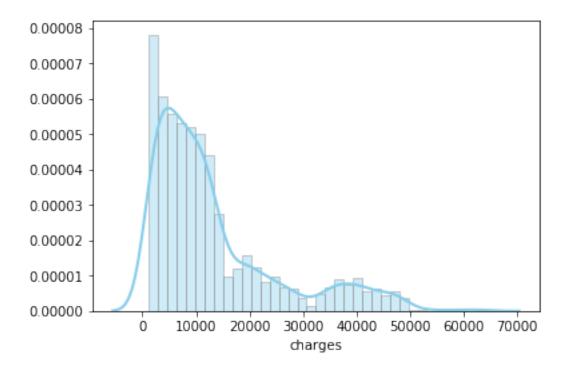
```
0 39.5 (14.1)
                                                          38.9 (14.1)
                                                                        0.446
                                                                               Two Sample
age, mean (SD)
                                             30.4 (6.0)
                                                           30.9 (6.1)
bmi, mean (SD)
                                                                        0.090
                                                                               Two Sample
children, n (%) 0
                                             289 (43.7)
                                                           285 (42.2)
                                                                        0.981
                                                                                      Chi-
                                             158 (23.9)
                                                           166 (24.6)
                 1
                 2
                                             119 (18.0)
                                                           121 (17.9)
                 3
                                              77 (11.6)
                                                            80 (11.8)
                 4
                                               11 (1.7)
                                                             14 (2.1)
                 5
                                                 8 (1.2)
                                                             10 (1.5)
smoker, n (%)
                                             547 (82.6)
                                                           517 (76.5)
                                                                        0.007
                                                                                      Chi-
                 no
                                             115 (17.4)
                 yes
                                                           159 (23.5)
                                             161 (24.3)
                                                           163 (24.1)
                                                                                      Chi-
region, n (%)
                 northeast
                                                                       0.933
                                             164 (24.8)
                                                           161 (23.8)
                 northwest
                                             175 (26.4)
                                                           189 (28.0)
                 southeast
                                             162 (24.5)
                                                           163 (24.1)
                 southwest
```

- [1] Warning, Hartigan's Dip Test reports possible multimodal distributions for: age.
- [2] Warning, test for normality reports non-normal distributions for: age.

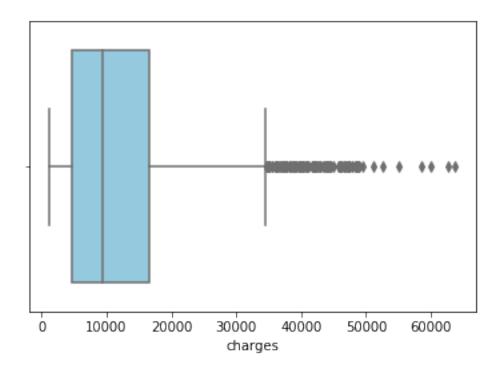
### 4.2 Descriptive analysis of the outcome variable charges

/Users/miaocai/anaconda3/lib/python3.7/site-packages/scipy/stats/stats.py:1713: FutureWarning: return np.add.reduce(sorted[indexer] \* weights, axis=axis) / sumval

Out[44]: <matplotlib.axes.\_subplots.AxesSubplot at 0x1a3997ec50>



```
In [45]: sns.boxplot(d['charges'], color = 'skyblue')
Out[45]: <matplotlib.axes._subplots.AxesSubplot at 0x1a39a7ce80>
```



In [46]: d['charges'].describe()

Out [46]:	count	1338.000000
	mean	13270.422265
	std	12110.011237
	min	1121.873900
	25%	4740.287150
	50%	9382.033000
	75%	16639.912515
	max	63770.428010

Name: charges, dtype: float64

#### 4.3 Cross-validation

Here I use the H20GeneralizedLinearEstimator module in h2o package to perform cross-validation. I set the number of cross-validation as 5 by nfolds=5, in which 6 models will be built. The first 5 models (cross-validation models) are built on 80% of the training data, and a different 20% is held out for each of the 5 models. Then the main model is built on 100% of the training data.

```
In [47]: target_var = 'charges'
         input_var = ['age', 'sex', 'bmi',
                      'children', 'smoker', 'region']
         glm_mod0 = \
             H20GeneralizedLinearEstimator(model_id = 'd_glm_0',
                                           family = 'gaussian',
                                           nfolds = 5,
                                           seed = 123)
         glm_mod0.train(x = input_var,
                        y = target_var,
                        training_frame = d0)
         glm_mod0.show()
glm Model Build progress: || 100%
Model Details
=========
H20GeneralizedLinearEstimator: Generalized Linear Modeling
Model Key: d_glm_0
ModelMetricsRegressionGLM: glm
** Reported on train data. **
MSE: 125728309.44330035
RMSE: 11212.863570172445
MAE: 8471.397911142334
RMSLE: 0.9331157151413909
R^2: 0.14203674139265943
Mean Residual Deviance: 125728309.44330035
Null degrees of freedom: 1337
Residual degrees of freedom: 1326
Null deviance: 196074221532.74988
Residual deviance: 168224478035.13586
AIC: 28776.289622947068
ModelMetricsRegressionGLM: glm
** Reported on cross-validation data. **
MSE: 129830749.84711617
RMSE: 11394.32972346843
MAE: 8600.97548619905
RMSLE: 0.9464119017196216
R^2: 0.11404190751089327
Mean Residual Deviance: 129830749.84711617
Null degrees of freedom: 1337
Residual degrees of freedom: 1326
Null deviance: 196632689167.88873
Residual deviance: 173713543295.44144
```

AIC: 28819.25062652632

Cross-Validation Metrics Summary:

	mean	sd	cv_1_valid	cv_2_valid	cv_3_valid	cv.
mae	8592.55	295.311	8582.31	7818.53	8785.11	87:
${\tt mean\_residual\_deviance}$	1.29276e+08	1.25685e+07	1.22953e+08	1.02176e+08	1.53851e+08	1.1
mse	1.29276e+08	1.25685e+07	1.22953e+08	1.02176e+08	1.53851e+08	1.1
null_deviance	3.93265e+10	4.53807e+09	3.72839e+10	2.96943e+10	4.90307e+10	3.
r2	0.110559	0.00589982	0.117462	0.114765	0.100491	0.:
residual_deviance	3.47427e+10	4.17128e+09	3.27055e+10	2.6157e+10	4.38475e+10	3.3
rmse	11342.6	557.598	11088.4	10108.2	12403.7	11:
rmsle	0.945845	0.0343231	0.981383	0.914074	0.884154	1.0

#### Scoring History:

timestamp	duration	iterations	negative_log_likelihood	objective
2019-05-12 22:43:32	0 000 sec	0	1.96074e+11	1 46543e+08

## 4.4 Machine learning

#### 4.4.1 Regularized regression

```
In [48]: from h2o.grid.grid_search import H2OGridSearch
         alpha_values = {'alpha': [0, 0.25, 0.5, 0.75, 1]}
         glm_mod2 = H2OGridSearch(
             H20GeneralizedLinearEstimator(family = 'gaussian',
                                           lambda_search = True,
                                            seed = 123), \setminus
         hyper_params = alpha_values)
         glm_mod2.train(x = input_var,
                        y = target_var,
                        training_frame = dtrain,
                       validation_frame = dvalid)
         glm_mod2.show()
glm Grid Build progress: || 100%
      alpha
                                                                 model_ids \
0
      [1.0] Grid_GLM_py_10_sid_929a_model_python_1557652172496_3_model_5
     [0.75] Grid_GLM_py_10_sid_929a_model_python_1557652172496_3_model_4
1
             Grid_GLM_py_10_sid_929a_model_python_1557652172496_3_model_3
```

```
3
     [0.25]
             Grid_GLM_py_10_sid_929a_model_python_1557652172496_3_model_2
      [0.0]
             Grid_GLM_py_10_sid_929a_model_python_1557652172496_3_model_1
       residual_deviance
     6.232294045221491E9
0
1 2.7448416102541004E10
2 2.7451841045226257E10
3 2.7452983289290577E10
4 2.7453233838145943E10
In [49]: glm_best = glm_mod2.get_grid()[0]
         glm_best._model_json['output']['coefficients_table'].as_data_frame()
Out [49]:
                                             standardized_coefficients
                               coefficients
         0
                    Intercept
                               -7206.776563
                                                           13492.999531
             region.northeast
                                  83.984427
                                                              83.984427
         1
         2
             region.northwest
                                 111.459665
                                                             111.459665
         3
             region.southeast
                                -192.376821
                                                            -192.376821
         4
             region.southwest
                                 -70.256674
                                                             -70.256674
         5
                    smoker.no -5020.292788
                                                           -5020.292788
         6
                   smoker.yes 18846.423625
                                                           18846.423625
         7
                   sex.female
                                 147.142857
                                                             147.142857
         8
                     sex.male
                               -142.895434
                                                            -142.895434
                                 255.041295
                                                            3604.495432
                          age
                                 329.352274
         10
                          bmi
                                                            2038.979286
         11
                     children
                                 477.291820
                                                             563.040100
In [50]: glm_best._model_json['output']['training_metrics']
ModelMetricsRegressionGLM: glm
** Reported on train data. **
MSE: 36244089.05252515
RMSE: 6020.306391914381
MAE: 4175.590832941357
RMSLE: NaN
R^2: 0.7557379707834732
Mean Residual Deviance: 36244089.05252515
```

Out [50]:

Null degrees of freedom: 955 Residual degrees of freedom: 944 Null deviance: 141853194478.7002 Residual deviance: 34649349134.21404

AIC: 19378.942718761107

```
In [51]: glm_best._model_json['output']['validation_metrics']
ModelMetricsRegressionGLM: glm
** Reported on validation data. **
MSE: 30107700.701553095
RMSE: 5487.04845081152
MAE: 3827.8094066015087
RMSLE: 0.5274009774363978
R^2: 0.7699240420817869
Mean Residual Deviance: 30107700.701553095
Null degrees of freedom: 206
Residual degrees of freedom: 195
Null deviance: 27453554523.254715
Residual deviance: 6232294045.221491
AIC: 4178.040900338396
Out [51]:
4.4.2 Auto-ML
In [52]: from h2o.automl.autoh2o import H2OAutoML
         autom1_1 = H2OAutoML(max_runtime_secs = 60)
         autom1_1.train(x = input_var,
                        y = target_var,
                        training_frame = dtrain,
                        validation_frame = dvalid)
         autom1_1.leaderboard
AutoML progress: || 100%
Out [52]:
In [53]: autom1_1.leader
Model Details
=========
H2OXGBoostEstimator : XGBoost
Model Key: XGBoost_grid_1_AutoML_20190512_224333_model_2
ModelMetricsRegression: xgboost
** Reported on train data. **
MSE: 14528508.374148928
```

RMSE: 3811.6280477177897 MAE: 2022.629675446195 RMSLE: 0.33941648050977435

Mean Residual Deviance: 14528508.374148928

ModelMetricsRegression: xgboost
\*\* Reported on validation data. \*\*

MSE: 18054575.204083566 RMSE: 4249.067568783011 MAE: 2344.0509905976373 RMSLE: 0.38510422313361437

Mean Residual Deviance: 18054575.204083566

ModelMetricsRegression: xgboost

\*\* Reported on cross-validation data. \*\*

MSE: 19784318.805394568 RMSE: 4447.956700035936 MAE: 2432.7904463891705 RMSLE: 0.41318440454888644

Mean Residual Deviance: 19784318.805394568

Cross-Validation Metrics Summary:

	mean	sd	cv_1_valid	cv_2_valid	cv_3_valid	cv.
mae	2432.73	74.7078	2490.93	2286.08	2333.17	248
mean_residual_deviance	1.97816e+07	1.54879e+06	2.23829e+07	1.95263e+07	1.74532e+07	1.
mse	1.97816e+07	1.54879e+06	2.23829e+07	1.95263e+07	1.74532e+07	1.
r2	0.864809	0.0109681	0.872214	0.836048	0.88118	0.8
residual_deviance	1.97816e+07	1.54879e+06	2.23829e+07	1.95263e+07	1.74532e+07	1.
rmse	4440.84	174.036	4731.05	4418.86	4177.71	416
rmsle	0.412534	0.0165132	0.403937	0.438595	0.418279	0.3

#### Scoring History:

timestamp	duration	number_of_trees	training_rmse	training_mae
2019-05-12 22:43:58	8.165 sec	0.0	18177.721142805927	13492.49952206152
2019-05-12 22:43:58	8.176 sec	5.0	14425.196741755824	10417.29248066028
2019-05-12 22:43:58	8.184 sec	10.0	11562.46886923096	8073.296127255491
2019-05-12 22:43:58	8.195 sec	15.0	9388.860994598781	6304.479055620138
2019-05-12 22:43:58	8.203 sec	20.0	7765.6711329633945	5018.130319252174
2019-05-12 22:43:58	8.333 sec	80.0	3900.143246524783	2049.8709798517584

2019-05-12 22:43:58	8.347 sec	85.0	3872.9667307722375	2046.128779455208
2019-05-12 22:43:58	8.361 sec	90.0	3851.652535206911	2031.336238334368
2019-05-12 22:43:58	8.376 sec	95.0	3828.628867905125	2024.791864498888
2019-05-12 22:43:58	8.392 sec	99.0	3811.6280477177897	2022.629675446195

See the whole table with table.as\_data\_frame() Variable Importances:

variable	relative_importance	scaled_importance	percentage	
smoker.no	4.54323e+11	1	0.55736	
		I		
bmi	1.48792e+11	0.327503	0.182537	
age	1.02772e+11	0.226209	0.12608	
smoker.yes	9.05798e+10	0.199373	0.111123	
children	8.18582e+09	0.0180176	0.0100423	
region.southeast	3.67247e+09	0.00808339	0.00450536	
region.northeast	2.91581e+09	0.00641794	0.0035771	
sex.female	1.9189e+09	0.00422366	0.0023541	
region.southwest	1.10821e+09	0.00243926	0.00135954	
sex.male	4.73685e+08	0.00104262	0.000581113	
region.northwest	3.91876e+08	0.000862549	0.000480751	

### Out[53]:

In [54]: autom1\_1.leader.cross\_validation\_metrics\_summary()

Cross-Validation Metrics Summary:

	mean	sd	cv_1_valid	cv_2_valid	cv_3_valid	cv.
mae	2432.73	74.7078	2490.93	2286.08	2333.17	248
mean_residual_deviance	1.97816e+07	1.54879e+06	2.23829e+07	1.95263e+07	1.74532e+07	1.
mse	1.97816e+07	1.54879e+06	2.23829e+07	1.95263e+07	1.74532e+07	1.
r2	0.864809	0.0109681	0.872214	0.836048	0.88118	0.8
residual_deviance	1.97816e+07	1.54879e+06	2.23829e+07	1.95263e+07	1.74532e+07	1.
rmse	4440.84	174.036	4731.05	4418.86	4177.71	416
rmsle	0.412534	0.0165132	0.403937	0.438595	0.418279	0.:

### Out [54]:

## 4.5 Neural networks using kera and tensorflow

```
from sklearn import preprocessing
         from sklearn.model_selection import train_test_split
         import matplotlib.pyplot as plt
         d = pd.read_csv("insurance.csv")
         col_types = d.dtypes.to_dict()
         col_types['age'] = 'float64'
         d = pd.read_csv("insurance.csv", dtype=col_types)
         d_dummy = pd.get_dummies(d, drop_first = True)
         y = d_dummy['charges'].values
         X = d_dummy.drop('charges', axis = 1).values
         X_train0, X_test0 = train_test_split(
             X, train_size = 0.8, random_state = 123)
         y_train0, y_test0 = train_test_split(
             y, train_size = 0.8, random_state = 123)
         X_train1, X_valid1 = train_test_split(
             X, train_size = 0.75, random_state = 123)
         y_train1, y_valid1 = train_test_split(
             y, train_size = 0.75, random_state = 123)
         # logistic regression
         def nn_model1():
             model = models.Sequential()
             model.add(layers.Dense(64, activation = 'relu',
                                   input_dim = X_train1.shape[1]))
             model.add(layers.Dense(1,
                                   activation = 'linear'))
             model.compile(optimizer = 'rmsprop',
                          loss = 'mse',
                          metrics = ['mae'])
             return model
         reg0 = nn_model1()
         reg0.fit(X_train1, y_train1, epochs = 200,
                  validation_data = [X_valid1, y_valid1],
                 verbose = 0)
/Users/miaocai/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_split.py:2179: F
  FutureWarning)
Out[55]: <keras.callbacks.History at 0x1a39ef4ef0>
In [56]: reg0.summary()
Layer (type)
                           Output Shape
                                                      Param #
```

from keras import optimizers

dense\_18 (Dense) (None, 64) 576

dense\_19 (Dense) (None, 1) 65

Total params: 641 Trainable params: 641 Non-trainable params: 0

\_\_\_\_\_\_

In [57]: reg0.history.history['loss'][199]

Out [57]: 125524612.95314057

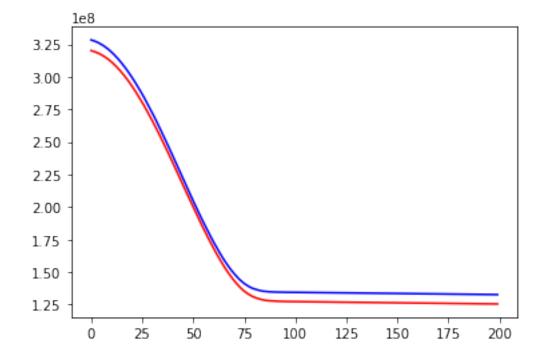
In [58]: reg0.history.history['val\_loss'][199]

Out [58]: 132704983.57014926

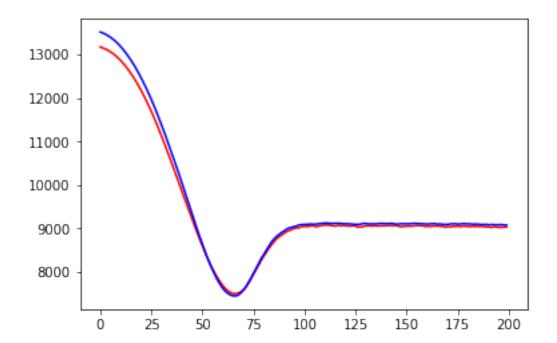
In [59]: reg0.history.history['val\_mean\_absolute\_error'][199]

Out [59]: 9081.118927821828

Out[60]: [<matplotlib.lines.Line2D at 0x1a3a48a470>]

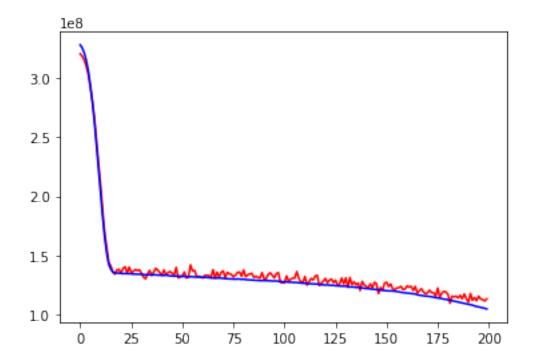


Out[61]: [<matplotlib.lines.Line2D at 0x1a3a4d5f60>]

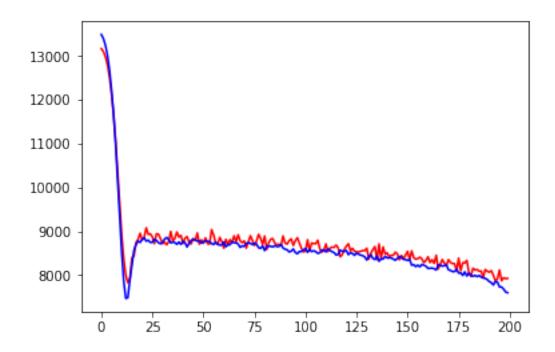


```
In [62]: def nn_model2():
             model = models.Sequential()
             model.add(layers.Dense(64, activation = 'relu',
                                   input_dim = X_train1.shape[1]))
             model.add(layers.Dropout(0.5))
             model.add(layers.Dense(64, activation = 'relu'))
             model.add(layers.Dropout(0.5))
             model.add(layers.Dense(1, activation = 'linear'))
             model.compile(optimizer = 'rmsprop',
                          loss = 'mse',
                          metrics = ['mae'])
             return model
         reg2 = nn_model2()
         reg2.fit(X_train1, y_train1, epochs = 200,
                  validation_data = [X_valid1, y_valid1],
                 verbose = 0)
Out[62]: <keras.callbacks.History at 0x1a3a4f16d8>
In [63]: plt.plot(reg2.history.history['loss'], color = 'red')
         plt.plot(reg2.history.history['val_loss'], color = 'blue')
```

Out[63]: [<matplotlib.lines.Line2D at 0x1a3a9d5748>]



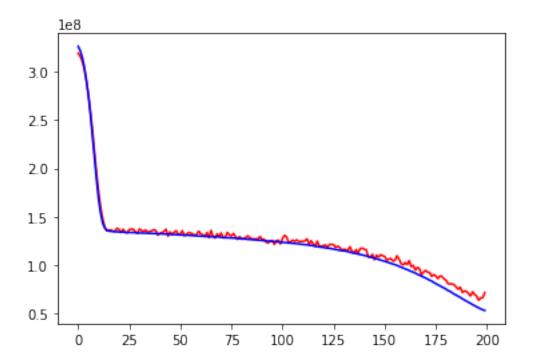
Out[64]: [<matplotlib.lines.Line2D at 0x1a3aa99e48>]



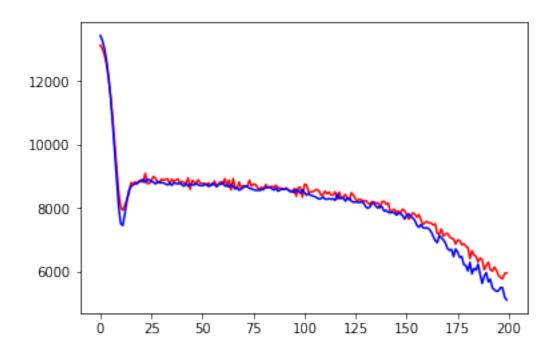
#### 4.5.1 A more complex model with dropout, L1 regularization, smaller weight

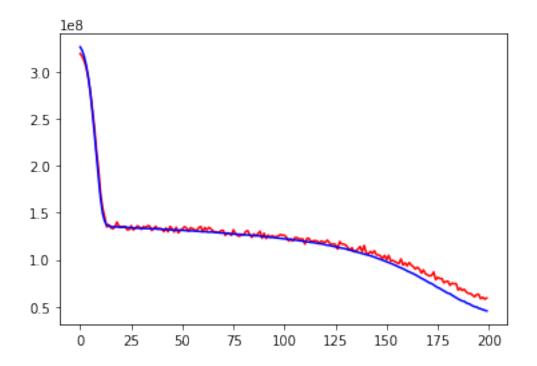
```
In [65]: from keras.regularizers import 11
      def nn_model3(l1_penalty):
         model = models.Sequential()
         model.add(layers.Dense(64, activation = 'relu',
                          kernel_regularizer =
                             11(11_penalty),
                         input_dim = X_train1.shape[1]))
         model.add(layers.Dropout(0.5))
         model.add(layers.Dense(64, activation = 'relu',
                         kernel_regularizer = l1(l1_penalty)))
         model.add(layers.Dropout(0.5))
         model.add(layers.Dense(1, activation = 'linear'))
         model.compile(optimizer = 'rmsprop',
                  loss = 'mse',
                  metrics = ['mae'])
         return model
In [66]: reg3 = nn_model3(0.1)
      reg3.fit(X_train1, y_train1, epochs = 200,
             validation_data = [X_valid1, y_valid1],
            verbose = 0)
      reg3.summary()
             Output Shape
Layer (type)
______
dense_23 (Dense)
                   (None, 64)
                                       576
_____
dropout_13 (Dropout) (None, 64)
-----
dense_24 (Dense)
                   (None, 64)
                                       4160
_____
dropout_14 (Dropout) (None, 64)
dense_25 (Dense) (None, 1)
                              65
______
Total params: 4,801
Trainable params: 4,801
Non-trainable params: 0
```

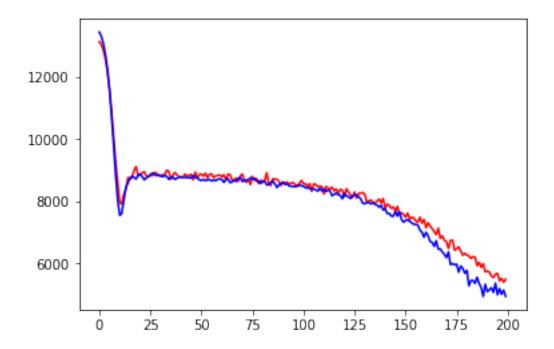
Out[67]: [<matplotlib.lines.Line2D at 0x1a3b03b128>]



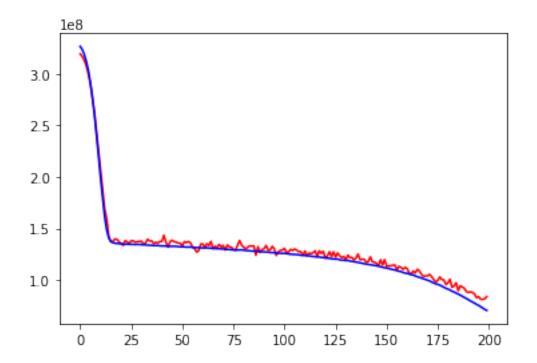
Out[68]: [<matplotlib.lines.Line2D at 0x1a3b0ffc50>]

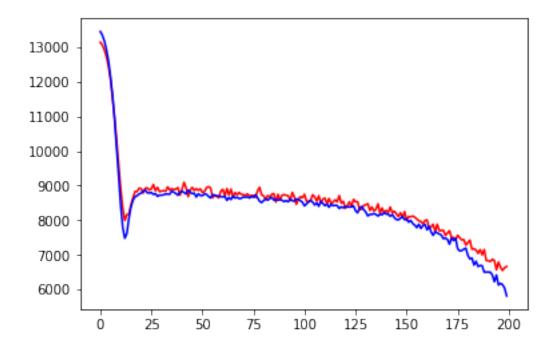






Out[71]: [<matplotlib.lines.Line2D at 0x1a23530470>]





## 5 Conclusion

Based on the machine learning and deep learning models used above, I found that using XGBoost provided in auto-ML tool provided by h2o tends to have the best model prediction performance. With regard to deep learning models, a two-layer neural network with L1 regularization seems to have the best prediction performance.