Concrete_Strength

November 11, 2018

1 Predicting Concrete Strength with Neural Networks

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1.1 Kaggle setup

Downloads data from https://www.kaggle.com/c/dat300-2018-concrete

```
In [1]: !pip install kaggle
```

```
Requirement already satisfied: kaggle in /usr/local/lib/python3.6/dist-packages (1.5.0)
Requirement already satisfied: urllib3<1.23.0,>=1.15 in /usr/local/lib/python3.6/dist-packages
Requirement already satisfied: python-slugify in /usr/local/lib/python3.6/dist-packages (from k
Requirement already satisfied: certifi in /usr/local/lib/python3.6/dist-packages (from kaggle)
Requirement already satisfied: six>=1.10 in /usr/local/lib/python3.6/dist-packages (from kaggle
Requirement already satisfied: tqdm in /usr/local/lib/python3.6/dist-packages (from kaggle) (4
Requirement already satisfied: python-dateutil in /usr/local/lib/python3.6/dist-packages (from
Requirement already satisfied: requests in /usr/local/lib/python3.6/dist-packages (from kaggle)
Requirement already satisfied: Unidecode>=0.04.16 in /usr/local/lib/python3.6/dist-packages (fr
Requirement already satisfied: idna<2.7,>=2.5 in /usr/local/lib/python3.6/dist-packages (from k
Requirement already satisfied: chardet<3.1.0,>=3.0.2 in /usr/local/lib/python3.6/dist-packages
```

```
In [2]: import io, os

        import googleapiclient.discovery
        import googleapiclient.http
        import google.colab

        def colab_kaggle_install_apikey():
          """
          Copies 'kaggle.json' from Google Drive to Colaboratory environment

          Based on https://medium.com/@move37timm/using-kaggle-api-for-google-colaboratory-d18
          """

          google.colab.auth.authenticate_user()
```

```
    drive_service = googleapiclient.discovery.build('drive', 'v3')
    results = drive_service.files().list(q="name = 'kaggle.json'", fields="files(id)").e
    kaggle_api_key = results.get('files', [])
    if len(kaggle_api_key) == 0:
      raise ValueError("Could not find kaggle.json in Google Drive")

    filename = "/root/.kaggle/kaggle.json"
    os.makedirs(os.path.dirname(filename), exist_ok=True)

    request = drive_service.files().get_media(fileId=kaggle_api_key[0]['id'])
    fh = io.FileIO(filename, 'wb')
    downloader = googleapiclient.http.MediaIoBaseDownload(fh, request)
    done = False
    while done is False:
        status, done = downloader.next_chunk()
    os.chmod(filename, 600)
    print('Installed to {}'.format(filename))

colab_kaggle_install_apikey()
```

```
Installed to /root/.kaggle/kaggle.json
```

In [3]:
```
!kaggle competitions download -c dat300-2018-concrete -p data/
```

```
Concrete_sampleSubmission.csv: Skipping, found more recently modified local copy (use --force
Concrete_test.csv: Skipping, found more recently modified local copy (use --force to force dow
Concrete_train.csv: Skipping, found more recently modified local copy (use --force to force do
```

In [0]:
```
import time

import pandas
import numpy
import matplotlib.pyplot as plt

import sklearn

import sklearn.preprocessing
import sklearn.model_selection
import sklearn.pipeline

import sklearn.linear_model
import sklearn.ensemble
import sklearn.svm

import keras
import keras.wrappers.scikit_learn
```

```
In [5]: dataset = pandas.read_csv('data/Concrete_train.csv')
        target_column = 'ConcreteCompressiveStrength'
        feature_columns = list(set(dataset.columns) - set([target_column]))

        dataset.head()
```

```
Out[5]:        Cement  BlastFurnaceSlag      FlyAsh       Water  Superplasticizer  \
        0  525.000000          0.000000    0.000000  189.000000               0.0
        1  276.000000        116.000000   90.000000  180.000000               9.0
        2  182.000000         45.200001  122.000000  170.199997               8.2
        3  212.600006          0.000000  100.400002  159.399994              10.4
        4  251.399994          0.000000  118.300003  188.500000               6.4

           CoarseAggregate  FineAggregate  Age  ConcreteCompressiveStrength
        0      1125.000000     613.000000    7                    42.419998
        1       870.000000     768.000000   28                    44.279999
        2      1059.400024     780.700012  100                    48.669998
        3      1003.799988     903.799988  100                    47.740002
        4      1028.400024     757.700012  100                    44.209999
```

```
In [8]: dataset.describe()
```

```
Out[8]:            Cement  BlastFurnaceSlag      FlyAsh       Water  Superplasticizer  \
        count  721.000000        721.000000  721.000000  721.000000        721.000000
        mean   277.400416         77.038835   56.515395  182.490569          6.051040
        std    104.586506         87.651090   65.031169   20.920979          5.660229
        min    102.000000          0.000000    0.000000  121.800003          0.000000
        25%    190.000000          0.000000    0.000000  167.000000          0.000000
        50%    254.000000         24.000000    0.000000  185.699997          6.100000
        75%    349.000000        145.000000  118.300003  192.000000         10.000000
        max    540.000000        359.399994  200.100006  247.000000         32.200001

               CoarseAggregate  FineAggregate         Age  ConcreteCompressiveStrength
        count       721.000000     721.000000  721.000000                   721.000000
        mean        971.709986     770.042163   44.049931                    35.321817
        std          77.788102      80.282289   60.614426                    16.706825
        min         801.000000     594.000000    1.000000                     2.330000
        25%         932.000000     724.299988    7.000000                    22.950001
        50%         968.000000     776.400024   28.000000                    33.950001
        75%        1028.400024     821.000000   56.000000                    45.080002
        max        1145.000000     992.599976  365.000000                    82.599998
```

1.2 Create models for comparisons

Baseline estimators from scikit-learn. Neural Networks using Keras with Tensorflow backend, using the scikit-learn estimator wrapper to have a compatible interface.

```
In [130]: def train_evaluate_model(X, Y, model, gridparams, gridcv=5, evalcv=5, test_size=0.3,
```

```
    scoring = 'neg_mean_absolute_error'
    metric = sklearn.metrics.mean_absolute_error

    X_train, X_test, Y_train, Y_test = \
      sklearn.model_selection.train_test_split(X, Y, test_size=test_size, random_sta


    # Find hyperparameters
    train_start = time.time()

    estimator = model
    if gridparams is None:
      details = None
    else:
      grid = sklearn.model_selection.GridSearchCV(model, gridparams, cv=gridcv, scor
                                                  iid=False, refit=False, return_tra
      grid.fit(X_train, Y_train)
      details = grid.cv_results_
      estimator.set_params(**grid.best_params_)


    # Fit with all training data
    history = estimator.fit(X_train, Y_train)
    if not getattr(history, 'history', None):
      history = None # only want the Keras History instances

    train_time = time.time() - train_start

    # Evaluate
    evaluate_start = time.time()
    train_score = metric(Y_train, estimator.predict(X_train))
    test_score = metric(Y_test, estimator.predict(X_test))
    evaluate_time =  time.time() - evaluate_start

    return test_score, history, details, train_time, evaluate_time, train_score, est

def build_mlp(layer_sizes, activation='relu'):
    Dense = keras.layers.Dense

    model = keras.Sequential()
    for i, size in enumerate(layer_sizes):
      params = dict(activation=activation)
      if i == 0:
        params['input_dim'] = 8
      model.add(Dense(size, **params))
      #print('i', size, i, params)
    model.add(Dense(1))
```

```
    optimizer = keras.optimizers.Adam(lr=0.001*5.0)

    model.compile(loss='mean_absolute_error', optimizer=optimizer)

    return model

def KerasMLP(layer_sizes, activation):
  def build_func():
    return build_mlp(layer_sizes, activation)

  early_stop = keras.callbacks.EarlyStopping(monitor='val_loss',
                                             min_delta=0.0, patience=50, verbose=0,
                                             mode='auto', baseline=None,
                                             restore_best_weights=True)

  reduce_lr = keras.callbacks.ReduceLROnPlateau(monitor='val_loss', factor=0.33,
                               patience=20, min_lr=0.0001, verbose=0)

  Wrapper = keras.wrappers.scikit_learn.KerasRegressor
  w = Wrapper(build_func, epochs=500, batch_size=50,
              callbacks=[reduce_lr], validation_split=0.25, verbose=0)
  return w

def PolyRidge(degree):
    m = sklearn.pipeline.make_pipeline(
      sklearn.preprocessing.PolynomialFeatures(degree),
      sklearn.linear_model.Ridge(),
    )
    return m

A_params = numpy.geomspace(0.001, 1000.0, 20)
C_params = numpy.geomspace(0.1, 1000.0, 12)
gamma_params = numpy.geomspace(0.01, 10.0, 12)

models = {
    'RandomForest': ( sklearn.ensemble.RandomForestRegressor(n_estimators=50),
                      {'max_depth': numpy.linspace(3, 50, 20)}),

    'MLP 64-32-16 tanh': ( KerasMLP([64,32,16],'tanh'), None ),

    #'MLP 16-8-4 Relu': ( KerasMLP([16,8,4],'relu'), None ),
    #'MLP 32-16-8 Relu': ( KerasMLP([32,16,8],'relu'), None ),
    'MLP 64-32-16 Relu': ( KerasMLP([64,32,16],'relu'), None ),
    #'MLP 128-64-32 Relu': ( KerasMLP([128,64,32],'relu'), None ),
    #'MLP 258-128-64 Relu': ( KerasMLP([256,128,64],'relu'), None ),
    'MLP 512-258-128 Relu': ( KerasMLP([512,256,128],'relu'), None ),
    'MLP 1024-512-256 Relu': ( KerasMLP([1024,512,256],'relu'), None ),
    'MLP 2048-1024-512 Relu': ( KerasMLP([2048,1024,512],'relu'), None ),
```

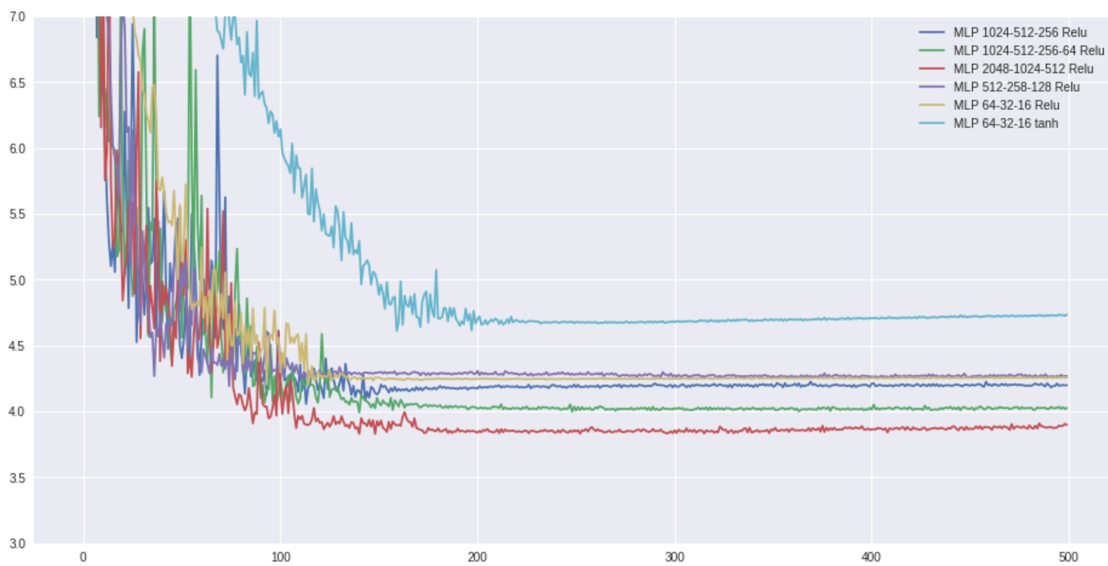
```python
        'MLP 1024-512-256-64 Relu': ( KerasMLP([1024,512,256,64],'relu'), None ),

        #'MLP wide 512-128 Relu': ( KerasMLP([512,128],'relu'), None ),
        #'MLP wide 1024-128 Relu': ( KerasMLP([1024,128],'relu'), None ),
        #'MLP wide 2048-256 Relu': ( KerasMLP([2048,256],'relu'), None ),
        #'MLP wide 2048-256 tanh': ( KerasMLP([2048,256],'tanh'), None ),

        #'MLP deep 128-128-128-32 Relu': ( KerasMLP([128,128,128,32],'relu'), None ),
        #'MLP deep 256-256-256-64 Relu': ( KerasMLP([256,256,256,64],'relu'), None ),

        'Poly4-Ridge': ( PolyRidge(4) , { 'ridge__alpha': A_params }),
        'Poly3-Ridge': ( PolyRidge(3) , { 'ridge__alpha': A_params }),
        'Poly2-Ridge': ( PolyRidge(2) , { 'ridge__alpha': A_params }),
        'Poly1-Ridge': ( PolyRidge(1) , { 'ridge__alpha': A_params }),

         # XXX: SVM, kernel=poly freezes when passing gamma
        'SVM linear': ( sklearn.svm.SVR(kernel='linear'), { 'C': C_params } ),
        'SVM poly3': ( sklearn.svm.SVR(kernel='poly', degree=3), { 'C': C_params } ),
        'SVM rbf': ( sklearn.svm.SVR(kernel='rbf'), { 'C': C_params, 'gamma': gamma_param
    }

    scaler = sklearn.preprocessing.StandardScaler()
    X = scaler.fit_transform(dataset[feature_columns])
    Y = dataset[target_column].values

    results = {}
    for i, model in enumerate(models.items()):
        name, values = model
        estimator, params = values
        print('training {}...'.format(name), end='')
        r = train_evaluate_model(X, Y, estimator, params)
        assert len(r) == 7, len(r)
        print('took {:1f} seconds. Test score: {:2f}'.format(r[3]+r[4], r[0]))
        results[name] = r
```

```
training RandomForest...took 11.035164 seconds. Test score: 4.241193
training MLP 64-32-16 tanh...took 35.818386 seconds. Test score: 4.450910
training MLP 64-32-16 Relu...took 35.861743 seconds. Test score: 4.406305
training MLP 512-258-128 Relu...took 55.518952 seconds. Test score: 4.023252
training MLP 1024-512-256 Relu...took 101.675818 seconds. Test score: 3.654873
training MLP 2048-1024-512 Relu...took 267.830899 seconds. Test score: 3.731886
training MLP 1024-512-256-64 Relu...took 104.819233 seconds. Test score: 3.679037
training Poly4-Ridge...took 6.462159 seconds. Test score: 6.259076
training Poly3-Ridge...took 2.131347 seconds. Test score: 5.433845
training Poly2-Ridge...took 0.699401 seconds. Test score: 6.678878
training Poly1-Ridge...took 0.319804 seconds. Test score: 8.676622
training SVM linear...took 20.341797 seconds. Test score: 9.253163
```

```
training SVM poly3...took 21.690072 seconds. Test score: 6.913316
training SVM rbf...took 31.874187 seconds. Test score: 4.604682
```

1.3 Plot learning progress of Neural Network

```
In [132]: val = { n : r[1].history['val_loss'] for n,r in results.items() if r[1] }
          def pad_to(length, v):
            a = numpy.full(length, numpy.nan)
            a[0:len(v)] = v
            return a

          longest = max([ len(v) for v in val.values() ])
          val = { k: pad_to(longest, v) for k,v in val.items() }
          val = pandas.DataFrame(val)
          val.plot(figsize=(16, 8), ylim=(3,7))

Out[132]: <matplotlib.axes._subplots.AxesSubplot at 0x7fa431bbf630>
```



Using `tanh` instead of `ReLu` activation converges significantly slower, and thus performs worse with same amount of training time. For that reason we focus on *ReLu*.

2 Summary of results

```
In [133]: def selected(r):
            # return a dictionary of data about the model selected by GridSearchCV
            cv_results = r[2]
            if cv_results is None:
              return {}
```

```
    df = pandas.DataFrame(cv_results)
    s = df.sort_values('rank_test_score', ascending=True)
    s = s.to_dict('rows')[0]
    return s

df = pandas.DataFrame({
    'model': list(results.keys()),
    'test_score': [ r[0] for r in results.values() ],
    'train_score': [ r[5] for r in results.values() ],
    'train_time': [ r[3] for r in results.values() ],
    'predict_time': [ r[4] for r in results.values() ],
    'params': [ selected(r).get('params', {}) for r in results.values() ],
})
df.sort_values(by='test_score', ascending=True)
```

Out[133]:

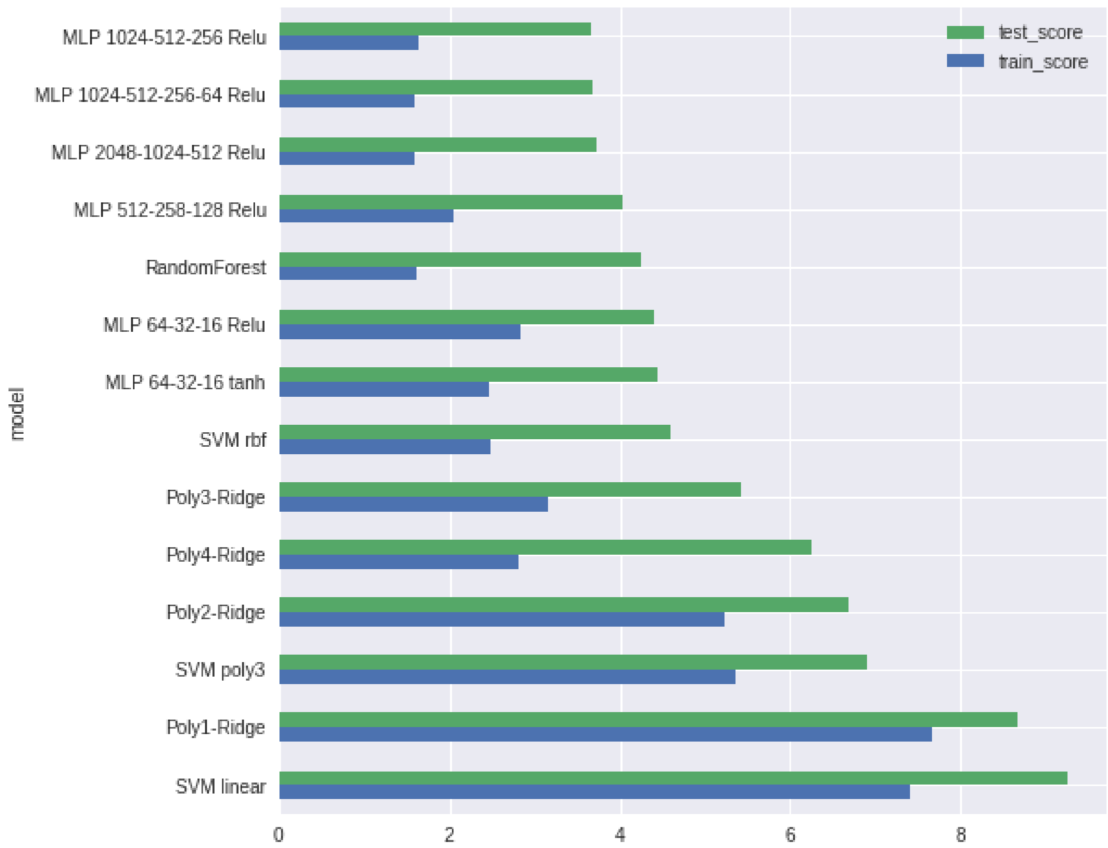
```
                        model  \
4      MLP 1024-512-256 Relu
6   MLP 1024-512-256-64 Relu
5     MLP 2048-1024-512 Relu
3       MLP 512-258-128 Relu
0               RandomForest
2          MLP 64-32-16 Relu
1          MLP 64-32-16 tanh
13                   SVM rbf
8                Poly3-Ridge
7                Poly4-Ridge
9                Poly2-Ridge
12                 SVM poly3
10               Poly1-Ridge
11                SVM linear

                                              params  predict_time  \
4                                                 {}      3.632936
6                                                 {}      3.708816
5                                                 {}      3.762365
3                                                 {}      3.562694
0                   {'max_depth': 37.631578947368425}      0.009444
2                                                 {}      3.519528
1                                                 {}      3.459194
13  {'C': 432.87612810830615, 'gamma': 0.065793322...      0.012139
8                  {'ridge__alpha': 1.438449888287663}      0.012279
7                 {'ridge__alpha': 26.366508987303554}      0.019643
9                  {'ridge__alpha': 1.438449888287663}      0.002223
12                            {'C': 35.11191734215131}      0.005360
10                            {'ridge__alpha': 0.001}      0.000665
11                                       {'C': 1000.0}      0.004122

    test_score  train_score  train_time
```

```
4      3.654873     1.628134    98.042882
6      3.679037     1.587300   101.110417
5      3.731886     1.592286   264.068533
3      4.023252     2.049588    51.956258
0      4.241193     1.619001    11.025720
2      4.406305     2.826139    32.342215
1      4.450910     2.454563    32.359193
13     4.604682     2.474714    31.862048
8      5.433845     3.157740     2.119068
7      6.259076     2.819240     6.442516
9      6.678878     5.223345     0.697177
12     6.913316     5.357967    21.684712
10     8.676622     7.665250     0.319139
11     9.253163     7.407687    20.337675
```

In [134]:
```python
desc = df.sort_values(by='test_score', ascending=False)
desc.plot(kind='barh',x='model', y=['train_score', 'test_score'], legend='reverse', i
```

```
/usr/local/lib/python3.6/dist-packages/pandas/plotting/_core.py:1716: UserWarning: Pandas doesn
  series.name = label
```

Out[134]: <matplotlib.axes._subplots.AxesSubplot at 0x7fa433ee02e8>



The baseline non-linear estimators RandomForest and SVM RBF got Mean-Absolute-Error (MAE) results of 4.2-4.6. Ridge linear regression on Polynomial features were unable to go under MAE 5.0. Pure linear models were unable to get under MAE 8.0. This suggest quite complex non-linear relationships between concrete strength and the contents of the concrete.

Generally bigger Neural Networks perform better. Both adding additional layers in depth, and increasing the size of layers increase the ability to represent the non-linearities of the system.

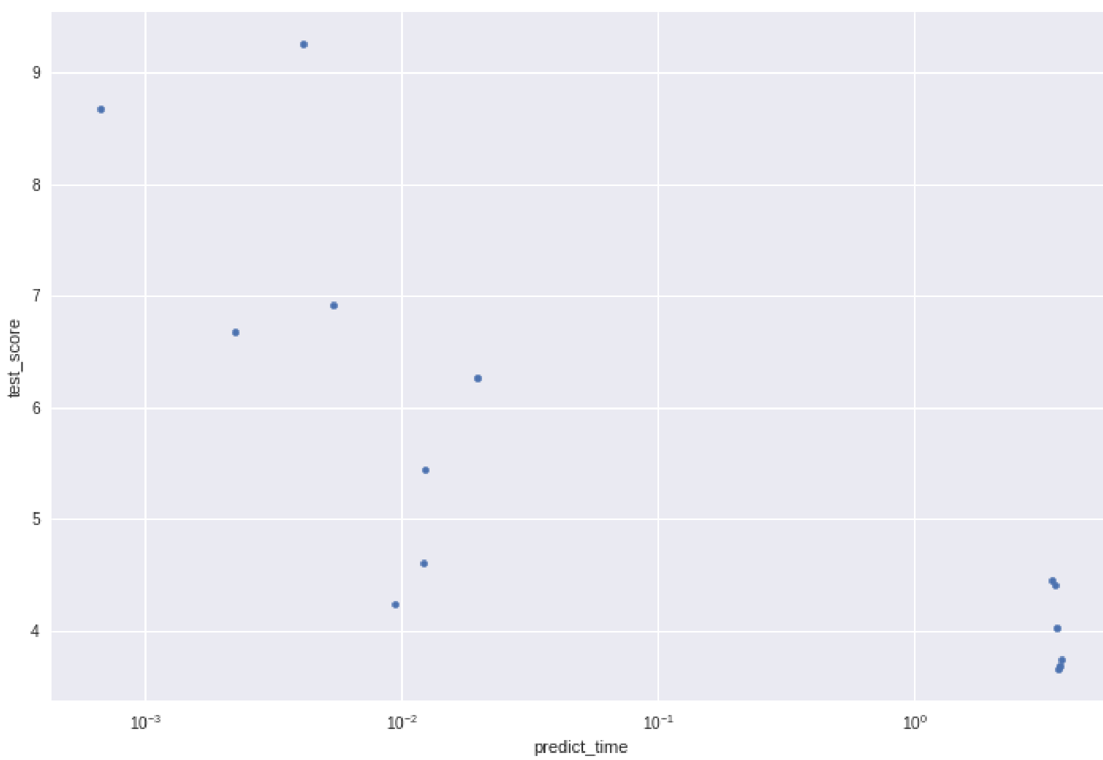
We were suprised by the number of neurons needed, especially considering that we only have 8 features. And that we were able to successfully train networks with over 1 million weights with only 900 instances in our dataset.

To reach MAE 3.6-3.7 with the Neural Networks, a critical addition was to use `ReduceLROnPlateau` to reduce learning rate. Before this, the learning progress was chaotic and noisy after epoch 100 (seemingly regardless of hyperparameters), and it was hard to get below MAE 4.0.

2.1 Accuracy versus inference time

```
In [142]: df.plot.scatter('predict_time', 'test_score', logx=True, figsize=(12, 8))
```

```
Out[142]: <matplotlib.axes._subplots.AxesSubplot at 0x7fa42f98def0>
```



The Neural Network methods are more than two orders-of-magnitude slower than the scikit-learn methods, even the networks that perform similarly to RandomForest and SVM RBF.

There is very little time difference between the smallest and largest neural networks, which suggest that there significant some constant-time overhead involved. Possibly this could be reduced by using the CPU for inference.

3 Kaggle submission

```
In [126]: import subprocess

          def make_submission(data, modelname, competition, submit=True):
            X_comp = scaler.transform(data[feature_columns])
            trained = results[modelname][6]
            Y_pred = trained.predict(X_comp)
            #print(X_comp.mean(axis=0), X_comp.std(axis=0))
            predictions = pandas.DataFrame({
                'ID': range(1, len(data)+1),
                'ConcreteCompressiveStrength': Y_pred,
            })
            print('means', predictions.ConcreteCompressiveStrength.mean(),
                  dataset.ConcreteCompressiveStrength.mean())

            filename = 'pred_{}.csv'.format(modelname.replace(' ', '_'))
            predictions.to_csv(filename, index=False, columns=['ID', 'ConcreteCompressiveStreng

            if submit:
              args = [
                  'kaggle', 'competitions', 'submit',
                  '-c', competition,
                  '-f', filename,
                  '-m', 'bla'
              ]
              try:
                out = subprocess.check_output(args)
              except subprocess.CalledProcessError as e:
                  print('error', e)
              print(out)

            return filename

          competeset = pandas.read_csv('data/Concrete_test.csv')
          make_submission(competeset, 'MLP 1024-512-256 Relu', 'dat300-2018-concrete')
```

```
means 37.26594 35.32181697919556
b'Successfully submitted to Concrete strength'
```

```
Out[126]: 'pred_MLP_1024-512-256_Relu.csv'
```

```
In [0]:
```