

```
In [3]: import numpy as np
import pandas as pd
from sklearn.model_selection import RandomizedSearchCV
from sklearn.metrics import mean_squared_error
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Conv1D, MaxPooling1D, Flatten
from tensorflow.keras.wrappers.scikit_learn import KerasRegressor
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
```

```
In [4]: parp_data = pd.read_csv('parp_merged.csv')
mtor_data = pd.read_csv('mtor_merged.csv')
akt_data = pd.read_csv('akt_merged.csv')

parp_data = parp_data.drop(columns=['Drug Name'])
mtor_data = mtor_data.drop(columns=['Drug Name'])
akt_data = akt_data.drop(columns=['Drug Name'])
combined_data = pd.concat([parp_data, mtor_data, akt_data])

features = combined_data.drop(columns=['Z Score'])
labels = combined_data['Z Score']
```

```
In [5]: scaler = StandardScaler()
features = scaler.fit_transform(features)

test_size = 0.1 #
train_features, test_features, train_labels, test_labels = train_test_split(features,
```

```
In [6]: def create_model(learning_rate=0.01, dropout_rate=0.2):
    model = Sequential()
    model.add(Conv1D(64, 3, activation='relu', input_shape=(2256, 1)))
    model.add(MaxPooling1D(2))
    model.add(Conv1D(128, 3, activation='relu'))
    model.add(MaxPooling1D(2))
    model.add(Conv1D(256, 3, activation='relu'))
    model.add(MaxPooling1D(2))
    model.add(Flatten())
    model.add(Dense(128, activation='relu'))
    model.add(Dense(64, activation='relu'))
    model.add(Dense(1))
    model.compile(optimizer='adam',
                  loss='mse',
                  metrics=['mae'])
    return model
```

```
In [7]: model = KerasRegressor(build_fn=create_model, verbose=0)

param_grid = {
    'learning_rate': [0.001, 0.01, 0.1],
    'batch_size': [16, 32, 64],
    'epochs': [50, 100, 150],
    'dropout_rate': [0.2, 0.3, 0.4]
}
```

```
C:\Users\mkapt\AppData\Local\Temp\ipykernel_19184\3930390662.py:1: DeprecationWarning: KerasRegressor is deprecated, use Sci-Keras (https://github.com/adriangb/scikeras) instead. See https://www.adriangb.com/scikeras/stable/migration.html for help migrating.
```

```
model = KerasRegressor(build_fn=create_model, verbose=0)
```

```
In [8]: random_search = RandomizedSearchCV(model, param_distributions=param_grid, n_iter=10,
      random_search.fit(train_features, train_labels)
      print("Best Hyperparameters:", random_search.best_params_)
```

```
Best Hyperparameters: {'learning_rate': 0.01, 'epochs': 150, 'dropout_rate': 0.2, 'batch_size': 64}
```

```
In [9]: best_model = random_search.best_estimator_
      test_features_resaped = test_features.reshape(-1, 2256, 1)
      test_predictions = best_model.predict(test_features_resaped)
      test_mse = mean_squared_error(test_labels, test_predictions)
      print("Test MSE:", test_mse)
```

```
Test MSE: 0.18832018977083637
```

```
In [14]: final_model = models.Sequential()
      final_model.add(layers.Conv1D(64, 3, activation='relu', input_shape=(2256, 1)))
      final_model.add(layers.MaxPooling1D(2))
      final_model.add(layers.Conv1D(128, 3, activation='relu'))
      final_model.add(layers.MaxPooling1D(2))
      final_model.add(layers.Conv1D(256, 3, activation='relu'))
      final_model.add(layers.MaxPooling1D(2))
      final_model.add(layers.Flatten())
      final_model.add(layers.Dense(128, activation='relu'))
      final_model.add(layers.Dense(64, activation='relu'))
      final_model.add(layers.Dense(1))

      final_model.compile(optimizer='adam',
                          loss='mse',
                          metrics=['mae'])
```

```
In [15]: epochs = 150
      final_model.fit(train_features, train_labels, epochs=epochs, batch_size=64)
```

Epoch 1/150
1/1 [=====] - 1s 873ms/step - loss: 1.9475 - mae: 1.2470
Epoch 2/150
1/1 [=====] - 0s 102ms/step - loss: 48.1490 - mae: 6.7376
Epoch 3/150
1/1 [=====] - 0s 100ms/step - loss: 0.3658 - mae: 0.4684
Epoch 4/150
1/1 [=====] - 0s 102ms/step - loss: 1.3881 - mae: 1.0182
Epoch 5/150
1/1 [=====] - 0s 102ms/step - loss: 1.2887 - mae: 0.9706
Epoch 6/150
1/1 [=====] - 0s 105ms/step - loss: 1.1053 - mae: 0.8779
Epoch 7/150
1/1 [=====] - 0s 115ms/step - loss: 0.9415 - mae: 0.7919
Epoch 8/150
1/1 [=====] - 0s 117ms/step - loss: 0.8224 - mae: 0.7287
Epoch 9/150
1/1 [=====] - 0s 110ms/step - loss: 0.7312 - mae: 0.6733
Epoch 10/150
1/1 [=====] - 0s 110ms/step - loss: 0.6615 - mae: 0.6248
Epoch 11/150
1/1 [=====] - 0s 122ms/step - loss: 0.5995 - mae: 0.5813
Epoch 12/150
1/1 [=====] - 0s 124ms/step - loss: 0.5338 - mae: 0.5398
Epoch 13/150
1/1 [=====] - 0s 110ms/step - loss: 0.4668 - mae: 0.4900
Epoch 14/150
1/1 [=====] - 0s 110ms/step - loss: 0.4067 - mae: 0.4462
Epoch 15/150
1/1 [=====] - 0s 108ms/step - loss: 0.3572 - mae: 0.4108
Epoch 16/150
1/1 [=====] - 0s 106ms/step - loss: 0.3230 - mae: 0.3971
Epoch 17/150
1/1 [=====] - 0s 108ms/step - loss: 0.3083 - mae: 0.4125
Epoch 18/150
1/1 [=====] - 0s 101ms/step - loss: 0.3126 - mae: 0.4322
Epoch 19/150
1/1 [=====] - 0s 99ms/step - loss: 0.3274 - mae: 0.4493
Epoch 20/150
1/1 [=====] - 0s 98ms/step - loss: 0.3390 - mae: 0.4587
Epoch 21/150
1/1 [=====] - 0s 97ms/step - loss: 0.3356 - mae: 0.4589
Epoch 22/150
1/1 [=====] - 0s 97ms/step - loss: 0.3149 - mae: 0.4432
Epoch 23/150
1/1 [=====] - 0s 99ms/step - loss: 0.2840 - mae: 0.4186
Epoch 24/150
1/1 [=====] - 0s 102ms/step - loss: 0.2535 - mae: 0.3924
Epoch 25/150
1/1 [=====] - 0s 102ms/step - loss: 0.2315 - mae: 0.3642
Epoch 26/150
1/1 [=====] - 0s 102ms/step - loss: 0.2203 - mae: 0.3423
Epoch 27/150
1/1 [=====] - 0s 103ms/step - loss: 0.2172 - mae: 0.3235
Epoch 28/150
1/1 [=====] - 0s 101ms/step - loss: 0.2158 - mae: 0.3153
Epoch 29/150
1/1 [=====] - 0s 105ms/step - loss: 0.2100 - mae: 0.3094
Epoch 30/150
1/1 [=====] - 0s 105ms/step - loss: 0.1980 - mae: 0.2999

Epoch 31/150
1/1 [=====] - 0s 109ms/step - loss: 0.1810 - mae: 0.2869
Epoch 32/150
1/1 [=====] - 0s 109ms/step - loss: 0.1617 - mae: 0.2737
Epoch 33/150
1/1 [=====] - 0s 106ms/step - loss: 0.1434 - mae: 0.2674
Epoch 34/150
1/1 [=====] - 0s 112ms/step - loss: 0.1285 - mae: 0.2630
Epoch 35/150
1/1 [=====] - 0s 105ms/step - loss: 0.1178 - mae: 0.2610
Epoch 36/150
1/1 [=====] - 0s 107ms/step - loss: 0.1101 - mae: 0.2563
Epoch 37/150
1/1 [=====] - 0s 101ms/step - loss: 0.1027 - mae: 0.2475
Epoch 38/150
1/1 [=====] - 0s 109ms/step - loss: 0.0930 - mae: 0.2352
Epoch 39/150
1/1 [=====] - 0s 98ms/step - loss: 0.0804 - mae: 0.2188
Epoch 40/150
1/1 [=====] - 0s 101ms/step - loss: 0.0665 - mae: 0.1972
Epoch 41/150
1/1 [=====] - 0s 100ms/step - loss: 0.0534 - mae: 0.1711
Epoch 42/150
1/1 [=====] - 0s 105ms/step - loss: 0.0435 - mae: 0.1445
Epoch 43/150
1/1 [=====] - 0s 103ms/step - loss: 0.0373 - mae: 0.1307
Epoch 44/150
1/1 [=====] - 0s 103ms/step - loss: 0.0331 - mae: 0.1332
Epoch 45/150
1/1 [=====] - 0s 111ms/step - loss: 0.0279 - mae: 0.1296
Epoch 46/150
1/1 [=====] - 0s 111ms/step - loss: 0.0210 - mae: 0.1159
Epoch 47/150
1/1 [=====] - 0s 113ms/step - loss: 0.0145 - mae: 0.0992
Epoch 48/150
1/1 [=====] - 0s 108ms/step - loss: 0.0107 - mae: 0.0870
Epoch 49/150
1/1 [=====] - 0s 108ms/step - loss: 0.0101 - mae: 0.0793
Epoch 50/150
1/1 [=====] - 0s 110ms/step - loss: 0.0107 - mae: 0.0763
Epoch 51/150
1/1 [=====] - 0s 108ms/step - loss: 0.0100 - mae: 0.0761
Epoch 52/150
1/1 [=====] - 0s 103ms/step - loss: 0.0083 - mae: 0.0749
Epoch 53/150
1/1 [=====] - 0s 104ms/step - loss: 0.0075 - mae: 0.0764
Epoch 54/150
1/1 [=====] - 0s 105ms/step - loss: 0.0084 - mae: 0.0786
Epoch 55/150
1/1 [=====] - 0s 99ms/step - loss: 0.0095 - mae: 0.0833
Epoch 56/150
1/1 [=====] - 0s 101ms/step - loss: 0.0093 - mae: 0.0821
Epoch 57/150
1/1 [=====] - 0s 109ms/step - loss: 0.0079 - mae: 0.0723
Epoch 58/150
1/1 [=====] - 0s 110ms/step - loss: 0.0068 - mae: 0.0605
Epoch 59/150
1/1 [=====] - 0s 104ms/step - loss: 0.0064 - mae: 0.0571
Epoch 60/150
1/1 [=====] - 0s 107ms/step - loss: 0.0060 - mae: 0.0577

Epoch 61/150
1/1 [=====] - 0s 104ms/step - loss: 0.0051 - mae: 0.0539
Epoch 62/150
1/1 [=====] - 0s 105ms/step - loss: 0.0037 - mae: 0.0459
Epoch 63/150
1/1 [=====] - 0s 106ms/step - loss: 0.0027 - mae: 0.0377
Epoch 64/150
1/1 [=====] - 0s 109ms/step - loss: 0.0024 - mae: 0.0370
Epoch 65/150
1/1 [=====] - 0s 116ms/step - loss: 0.0024 - mae: 0.0375
Epoch 66/150
1/1 [=====] - 0s 118ms/step - loss: 0.0024 - mae: 0.0362
Epoch 67/150
1/1 [=====] - 0s 112ms/step - loss: 0.0021 - mae: 0.0356
Epoch 68/150
1/1 [=====] - 0s 110ms/step - loss: 0.0019 - mae: 0.0353
Epoch 69/150
1/1 [=====] - 0s 104ms/step - loss: 0.0019 - mae: 0.0368
Epoch 70/150
1/1 [=====] - 0s 110ms/step - loss: 0.0021 - mae: 0.0391
Epoch 71/150
1/1 [=====] - 0s 109ms/step - loss: 0.0023 - mae: 0.0403
Epoch 72/150
1/1 [=====] - 0s 108ms/step - loss: 0.0023 - mae: 0.0399
Epoch 73/150
1/1 [=====] - 0s 106ms/step - loss: 0.0021 - mae: 0.0381
Epoch 74/150
1/1 [=====] - 0s 104ms/step - loss: 0.0020 - mae: 0.0352
Epoch 75/150
1/1 [=====] - 0s 102ms/step - loss: 0.0019 - mae: 0.0328
Epoch 76/150
1/1 [=====] - 0s 104ms/step - loss: 0.0019 - mae: 0.0311
Epoch 77/150
1/1 [=====] - 0s 107ms/step - loss: 0.0017 - mae: 0.0296
Epoch 78/150
1/1 [=====] - 0s 112ms/step - loss: 0.0015 - mae: 0.0275
Epoch 79/150
1/1 [=====] - 0s 111ms/step - loss: 0.0013 - mae: 0.0255
Epoch 80/150
1/1 [=====] - 0s 120ms/step - loss: 0.0011 - mae: 0.0236
Epoch 81/150
1/1 [=====] - 0s 131ms/step - loss: 0.0011 - mae: 0.0226
Epoch 82/150
1/1 [=====] - 0s 112ms/step - loss: 0.0010 - mae: 0.0217
Epoch 83/150
1/1 [=====] - 0s 107ms/step - loss: 9.7320e-04 - mae: 0.0193
Epoch 84/150
1/1 [=====] - 0s 111ms/step - loss: 9.0389e-04 - mae: 0.0176
Epoch 85/150
1/1 [=====] - 0s 107ms/step - loss: 8.8504e-04 - mae: 0.0172
Epoch 86/150
1/1 [=====] - 0s 102ms/step - loss: 9.2092e-04 - mae: 0.0186
Epoch 87/150
1/1 [=====] - 0s 102ms/step - loss: 9.6229e-04 - mae: 0.0198
Epoch 88/150
1/1 [=====] - 0s 102ms/step - loss: 9.6640e-04 - mae: 0.0202
Epoch 89/150
1/1 [=====] - 0s 100ms/step - loss: 9.4093e-04 - mae: 0.0197
Epoch 90/150
1/1 [=====] - 0s 105ms/step - loss: 9.2248e-04 - mae: 0.0185

Epoch 91/150
1/1 [=====] - 0s 104ms/step - loss: 9.2578e-04 - mae: 0.0176
Epoch 92/150
1/1 [=====] - 0s 103ms/step - loss: 9.2959e-04 - mae: 0.0173
Epoch 93/150
1/1 [=====] - 0s 100ms/step - loss: 9.1040e-04 - mae: 0.0166
Epoch 94/150
1/1 [=====] - 0s 103ms/step - loss: 8.7397e-04 - mae: 0.0160
Epoch 95/150
1/1 [=====] - 0s 119ms/step - loss: 8.4560e-04 - mae: 0.0161
Epoch 96/150
1/1 [=====] - 0s 110ms/step - loss: 8.3778e-04 - mae: 0.0160
Epoch 97/150
1/1 [=====] - 0s 106ms/step - loss: 8.3872e-04 - mae: 0.0156
Epoch 98/150
1/1 [=====] - 0s 107ms/step - loss: 8.3202e-04 - mae: 0.0153
Epoch 99/150
1/1 [=====] - 0s 118ms/step - loss: 8.1762e-04 - mae: 0.0149
Epoch 100/150
1/1 [=====] - 0s 121ms/step - loss: 8.0843e-04 - mae: 0.0142
Epoch 101/150
1/1 [=====] - 0s 113ms/step - loss: 8.1110e-04 - mae: 0.0143
Epoch 102/150
1/1 [=====] - 0s 105ms/step - loss: 8.1800e-04 - mae: 0.0149
Epoch 103/150
1/1 [=====] - 0s 107ms/step - loss: 8.1809e-04 - mae: 0.0151
Epoch 104/150
1/1 [=====] - 0s 104ms/step - loss: 8.1071e-04 - mae: 0.0148
Epoch 105/150
1/1 [=====] - 0s 110ms/step - loss: 8.0405e-04 - mae: 0.0141
Epoch 106/150
1/1 [=====] - 0s 105ms/step - loss: 8.0303e-04 - mae: 0.0140
Epoch 107/150
1/1 [=====] - 0s 106ms/step - loss: 8.0368e-04 - mae: 0.0141
Epoch 108/150
1/1 [=====] - 0s 104ms/step - loss: 7.9999e-04 - mae: 0.0139
Epoch 109/150
1/1 [=====] - 0s 104ms/step - loss: 7.9226e-04 - mae: 0.0133
Epoch 110/150
1/1 [=====] - 0s 108ms/step - loss: 7.8600e-04 - mae: 0.0128
Epoch 111/150
1/1 [=====] - 0s 104ms/step - loss: 7.8421e-04 - mae: 0.0128
Epoch 112/150
1/1 [=====] - 0s 107ms/step - loss: 7.8413e-04 - mae: 0.0128
Epoch 113/150
1/1 [=====] - 0s 127ms/step - loss: 7.8204e-04 - mae: 0.0126
Epoch 114/150
1/1 [=====] - 0s 123ms/step - loss: 7.7830e-04 - mae: 0.0122
Epoch 115/150
1/1 [=====] - 0s 112ms/step - loss: 7.7617e-04 - mae: 0.0119
Epoch 116/150
1/1 [=====] - 0s 104ms/step - loss: 7.7683e-04 - mae: 0.0117
Epoch 117/150
1/1 [=====] - 0s 102ms/step - loss: 7.7803e-04 - mae: 0.0117
Epoch 118/150
1/1 [=====] - 0s 119ms/step - loss: 7.7749e-04 - mae: 0.0117
Epoch 119/150
1/1 [=====] - 0s 121ms/step - loss: 7.7581e-04 - mae: 0.0116
Epoch 120/150
1/1 [=====] - 0s 105ms/step - loss: 7.7498e-04 - mae: 0.0116

Epoch 121/150
1/1 [=====] - 0s 107ms/step - loss: 7.7536e-04 - mae: 0.0115
Epoch 122/150
1/1 [=====] - 0s 114ms/step - loss: 7.7542e-04 - mae: 0.0116
Epoch 123/150
1/1 [=====] - 0s 106ms/step - loss: 7.7415e-04 - mae: 0.0114
Epoch 124/150
1/1 [=====] - 0s 106ms/step - loss: 7.7240e-04 - mae: 0.0112
Epoch 125/150
1/1 [=====] - 0s 113ms/step - loss: 7.7146e-04 - mae: 0.0110
Epoch 126/150
1/1 [=====] - 0s 111ms/step - loss: 7.7130e-04 - mae: 0.0110
Epoch 127/150
1/1 [=====] - 0s 114ms/step - loss: 7.7095e-04 - mae: 0.0109
Epoch 128/150
1/1 [=====] - 0s 116ms/step - loss: 7.7006e-04 - mae: 0.0107
Epoch 129/150
1/1 [=====] - 0s 109ms/step - loss: 7.6931e-04 - mae: 0.0104
Epoch 130/150
1/1 [=====] - 0s 104ms/step - loss: 7.6930e-04 - mae: 0.0105
Epoch 131/150
1/1 [=====] - 0s 111ms/step - loss: 7.6966e-04 - mae: 0.0106
Epoch 132/150
1/1 [=====] - 0s 111ms/step - loss: 7.6972e-04 - mae: 0.0105
Epoch 133/150
1/1 [=====] - 0s 109ms/step - loss: 7.6941e-04 - mae: 0.0104
Epoch 134/150
1/1 [=====] - 0s 110ms/step - loss: 7.6922e-04 - mae: 0.0105
Epoch 135/150
1/1 [=====] - 0s 106ms/step - loss: 7.6932e-04 - mae: 0.0105
Epoch 136/150
1/1 [=====] - 0s 101ms/step - loss: 7.6939e-04 - mae: 0.0105
Epoch 137/150
1/1 [=====] - 0s 106ms/step - loss: 7.6913e-04 - mae: 0.0104
Epoch 138/150
1/1 [=====] - 0s 108ms/step - loss: 7.6870e-04 - mae: 0.0103
Epoch 139/150
1/1 [=====] - 0s 111ms/step - loss: 7.6846e-04 - mae: 0.0102
Epoch 140/150
1/1 [=====] - 0s 119ms/step - loss: 7.6842e-04 - mae: 0.0102
Epoch 141/150
1/1 [=====] - 0s 110ms/step - loss: 7.6835e-04 - mae: 0.0102
Epoch 142/150
1/1 [=====] - 0s 119ms/step - loss: 7.6815e-04 - mae: 0.0101
Epoch 143/150
1/1 [=====] - 0s 122ms/step - loss: 7.6800e-04 - mae: 0.0100
Epoch 144/150
1/1 [=====] - 0s 122ms/step - loss: 7.6804e-04 - mae: 0.0100
Epoch 145/150
1/1 [=====] - 0s 121ms/step - loss: 7.6814e-04 - mae: 0.0100
Epoch 146/150
1/1 [=====] - 0s 121ms/step - loss: 7.6815e-04 - mae: 0.0100
Epoch 147/150
1/1 [=====] - 0s 121ms/step - loss: 7.6807e-04 - mae: 0.0100
Epoch 148/150
1/1 [=====] - 0s 108ms/step - loss: 7.6803e-04 - mae: 0.0100
Epoch 149/150
1/1 [=====] - 0s 121ms/step - loss: 7.6805e-04 - mae: 0.0100
Epoch 150/150
1/1 [=====] - 0s 124ms/step - loss: 7.6803e-04 - mae: 0.0100

Out[15]: <keras.callbacks.History at 0x254bccface0>

```
In [16]: evaluation = final_model.evaluate(test_features, test_labels)
print("Final Evaluation Loss:", evaluation[0])
print("Final Evaluation MAE:", evaluation[1])
```

```
1/1 [=====] - 0s 131ms/step - loss: 0.1901 - mae: 0.4230
Final Evaluation Loss: 0.19013060629367828
Final Evaluation MAE: 0.4229690432548523
```

```
In [17]: predictions = final_model.predict(test_features)
print("Predictions:", predictions)
```

```
1/1 [=====] - 0s 73ms/step
Predictions: [[-1.0103655]
              [-1.3365492]]
```

```
In [18]: final_model.save("drug_response_prediction_model.h5")
```