CS 181 Practical Writeup

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1 Introduction

Our approach to predicting the HOMO-LUMO gap employed linear regression methods, random forests, and neural networks. We found that a random forest regressor performed moderately well relative to the class and that there were opportunities for further improvement of the basic model by increasing the number of predictors from RDkit's fingerprinting feature [5]. In all of these models, due to time and computational power constraints, we trained on data from the first 50,000 molecules and used subsequent sets of 50,000 molecules as validation sets.

2 Basic Regression Techniques

2.1 Initial Runs

We first utilized the benchmark techniques: simple linear regression and ridge regression with the default coefficient weight for the penalty term (α) of 0.5. When running these on our 50,000 molecule sample sets, we obtained RMSE values of .29820072 and .29818009, respectively. We also ran these regression techniques in the Kaggle competition, and based on those results, we concluded that the 50,000 molecule sample yielded accuracy scores sufficiently similar to the actual test data, and differences in performance of separate techniques was especially sufficiently reflective of differences in test data performance between those techniques.

2.2 Ridge Regression Cross Validation

We used a standard cross validation approach, as has been discussed in section, in order to determine an optimal alpha value for ridge regression. To do this, we utilized the scikit-learn RidgeCV function [6]. This yielded an alpha value of 1.175; however, the performance with this alpha value was relatively negligible in comparison to the default ridge regression, reflecting inherent complexity in the data that could not be modeled using the ridge regression technique.

2.3 Lasso Regression and Elastic Net Regularization

Similar issues were encountered when trying lasso regression. In comparison to ridge regression, lasso regression tends to deselects some features by driving their weight in the regression to 0 as the alpha parameter is increased. We used the Elastic Net method, which allows for a mixture between ridge and lasso by minimizing the same least squares expression as ridge and lasso, but with penalty term of $\frac{\alpha(1-\rho)}{2}\sum_1^J |w_j|^2 + \frac{\alpha\rho}{2}\sum_1^J |w_j|$, for $0 \leq \rho \leq 1$.

We found that the model, under cross validation of the alpha and rho parameters using ElasticNetCV, chose a rho of 0, which corresponds to completing favoring ridge regression. As expected, the optimal alpha value was 1.175, the same as under testing with RidgeCV.

3 Random Forest Regression

3.1 Background

Next we consider the random forest regression method, which is an ensemble algorithm that is quite efficient yet often quite accurate for large data sets [7]. It employs a decision tree classification idea and averages performance over numerous decision trees. Each decision tree uses a random sample of the training data (drawn with replacement). To complete the classification within each tree, one completes a series of binary splits which divides the data

subsequently into groups. For each split, a random sample of features is compared. For each feature, one optimizes the residual sum of squares; that is, one picks the value that creates two groups (above [A] and below [B] the value) such that the expression $\sum_A (y_A - \mu_A)^2 + \sum_B (y_B - \mu_B)^2$ is minimized, where μ_A, μ_B are the respective means of the two groups. Then, take the minimum of this number over all the features to use as the split. At the end, the value assigned to each leaf node group is the average of the target values for the members of that group. Given the regressor, categorizing test data just amounts to following each tree down through the splits, and then averaging the values obtained from the resulting leaf node group of each decision tree. [8] [9]

One parameter to set through testing is the number of features that are randomly chosen to be compared at each split. Also, the greater the depth of the trees utilized before stopping the procedure, the smaller the bias; however, this requires a much higher number of trees (another parameter) in order to maintain relatively low variance. Higher numbers of trees will generate more accurate predictions, but with diminishing returns.

3.2 Model Selection

Upon investigating different max number of features to select from at each split, we found there to be very small difference between using the square root of the number of features, the base-2 log of the number of features, and our scikit-learn function RandomForestRegressor's default setting of using all features. We ultimately worked with the square root, which gave the (marginally) best RMSE error in our tests. We changed the default setting of using 10 decision trees in the random forest to using 300 trees, after our tests revealed diminishing returns to increasing the number of trees at around 300, but somewhat significant improvements up until that point. See graph in Figure 1 (on the last page of the document).

3.3 Error Analysis and Post-Prediction Adjustments

Using 50,000 molecules as the training set and 50,000 molecules as the test set with the random forest model yielded a RMSE of about .276. To analyze this error, we plotted Actual Gap Value vs. Error (Actual - Predicted Value) [Figure 2] and Predicted Gap Value vs. Error (Actual - Predicted Value) [Figure 3]. From Figure 2, we see that our random forest is consistently underestimating high gap values and overestimating low gap values; that is, the predictions are not extreme enough, mainly instead staying around the mean. Such underfitting is also reflected in how RMSE on train and test data is about the same and in how taking the average of predictions for random forests and ridge regression, a mixture as in the Netflix Prize approaches, was unsuccessful (the two models underfit in the same direction).

However, we don't know the actual values when doing an actual prediction. Unfortunately, as shown in Figure 3, we cannot make out as much of a pattern when considering only observed prediction values. We can still artificially correct for this small amount of error, however, by fitting a polynomial curve to the Figure 3 data. Then, given actual test data, we can make our prediction using random forest and then add on the correction number as given by the polynomial for each prediction value to reduce the RMSE. This depends on using the same training data to generate the regressor for the validation data (which generates the polynomial) and the actual test data.

With 50,000 molecule training and validation sets, we fit polynomials (Degree 2, 3, and 5 shown in Figures 4-6). Based on tail behavior and overfitting to outliers in the data, we used the cubic $-0.09511856x^3 + 0.53458563x^2 - 0.98841412x + 0.60673527$ to compute corrections. Testing on a third set of 50,000 molecules yielded sizably better RMSE scores than without the adjustment.

3.4 Training Set Size's Impact on Error

To make our best predictions on the actual test data, we needed to use a random forest trained on a much larger amount of the given 824,230 molecules. With a new training set, we also need a new validation set to determine a polynomial for the adjustment. Thus we used 700,000 molecules to train the random forest and the remaining 124,230 molecules to determine a polynomial. Unfortunately, we did not previously anticipate that this time, the polynomial generated negligible corrections for predictions, and thus RMSE was only very slightly better (about .00001) than for just the random forest regressor on its own. [Figure 7] In fact, a better RMSE could be obtained by simply using all 824,230 molecules as training data; the benefit of more training data eclipsed that of the polynomial correction. We thus conclude that the polynomial correction previously worked because the training sample size was too small to fully capture the power of random forests; with enough training data, the random forest's predictions are unbiased. After that, there is simply an inherent limit to the ability for random forests to make good predictions on this data.

4 Artificial Neural Network Regression

4.1 Background

Artificial neural networks (ANN) are a set of biologically inspired algorithms for machine learning. There is a neural network net, composed of a set of input nodes in the first layer, hidden nodes (in zero or more hidden layers), and output notes in the last layer. All the nodes in one layer are connected to all the nodes in the next layer. A neural network takes in a vector as input (each node takes an element of the vector). Then, the nodes fire based on an activation function: for a non-linear activation function such as the sigmoid or hyperbolic tangent, each node will send a signal to its connections based on how large or small the input to them was. Each node in the second layer collects all of the inputs from the previous layer and weighs them linearly by weights on the connections, and then fires again according to the activation function to the third layer. Finally, the output layer will have the output of the neural network; for a regression problem like this, there is one output node which will output a value, a weighted linear combination of the nodes that fired in the previous layer. [1]

Most of the work done in artificial neural networks research involves the creation of learning algorithms to optimize the weights between nodes. [3]

4.2 Setting up an ANN

We decided to use the Torch7 machine learning library to create and train an artificial neural network [2]. Installing and setting up dependencies took a rather long time. Ultimately, we were able to run Torch7 on Ubuntu 14.04 LTS on a 4.0GHz Intel i7 processor and a Nvidia GeForce GTX 750 Ti graphics card with GPU acceleration. Training a neural network on the GPU rather than the CPU resulted in five to twenty time speedups, well worth the initial time investment in setting up the dependencies.

4.3 Training algorithm

The training algorithm is where the optimization of the neural network occurred and the "heart" of the machine learning. We implemented a simple backpropagation algorithm that involved gradient descent. In preparation for this, we used a tanh activation function for all of the nodes (to use gradient descent, the activation function has to be differentiable). The backpropagation algorithm sends error signals backwards through the neural network to update the weights to minimize the error loss function, which we defined as the mean squared error. Minimizing the mean squared error is the same as minimizing our root mean squared error. [4]

4.4 Desiging our ANN

Initially, we designed the neural network with 256 input nodes (one for each element in the feature vector), and 1 output node (for the output). We trained it for 100 iterations on the first 10,000 rows of the data, and then tested its performance on the second 10,000 rows of the data. This resulted in a RMSE error of around 0.2994. Without a hidden layer, the neural network almost does the same thing as linear regression: it takes the feature vector, performs some linear operation to it, then performs a nonlinear operation (tanh) and then returns an answer. To do better learning, we would have to add a hidden layer to the ANN.

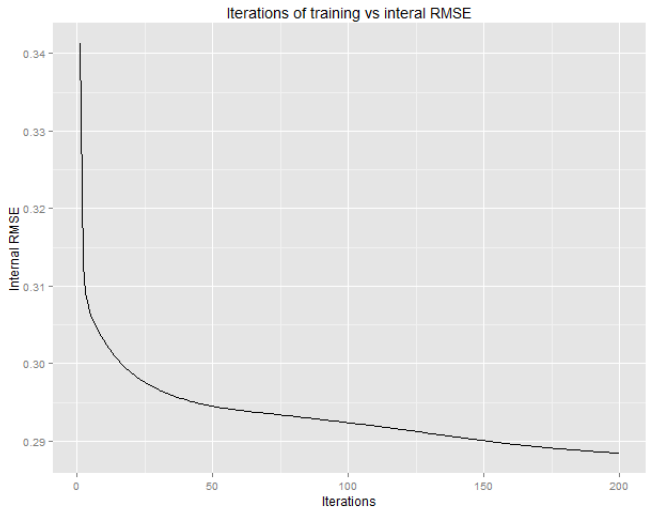
Now, the problem at hand was finding a good structure for the neural network. We experimented with 32, 64, 128, 256, 512, and 1024 hidden layers, using 3-fold cross validation for a total set of 30,000 random rows (same rows for each test, this took us a few hours). Below is a table of the RMSE after training for 200 iterations and a learning rate of 0.01:

Nodes in hidden layer	Average RMSE of the model
32	0.29403
64	0.29489
128	0.29319
256	0.29314
512	0.29296
1024	0.29342

Unfortunately, we were unable to differentiate between the performance of different numbers of hidden nodes because of how close the RMSE values are to each other. In general, there should be a balance between too few nodes (underfitting) and too many nodes (overfitting), but we did not notice either underfitting or overfitting. However, in an experiment on a smaller set of the data, a 3-fold cross-validation on a total of 300 randomly chosen elements, we found a lot of overfitting as the number of nodes increased.

To better understand how the training algorithm performed, we can look at a graph of the internal root mean squared error of the model during training at each iteration of the stochastic gradient descent algorithm. In the end, we worked mostly with the neural network with 128 hidden nodes for speed purposes.

The main bottleneck that we faced was time: at 200 iterations, it seems as if the curve, the internal RMSE, levels off and does not decrease very much. After around 600 iterations (we did not record the internal data for this, only the end result), the internal RMSE was 0.27711, showing diminishing marginal returns. The interal RMSE is a lower bound on the performance of any model on new data, so we chose not to proceed with the neural network model in the interest of time and efficiency.



4.5 Results and conclusion for ANNs

With our neural network structure, we were unable to see any large improvements over the simple ridge linear regression method. We suspect that this may have been due to the quality of the data - our neural networks seemed to have a difficult time predicting values even with a good training algorithm. Perhaps the features of the smiles string do not correlate very much with the energy gap. If we had more time, we would have went into RDKit to extract more relevant features that may pertain more to the energy gap and train the neural network on these larger vectors. Determining which elements of the features vector to keep and which not to keep would also help in a neural networks approach.

4.6 Further work

It's almost time to submit this report (11:00PM), but we actually attempted some of our own suggestions in the above section. Using RDKit, we extracted 512-bit feature vectors for the molecules and trained a new ANN with them. The new ANN has 512 inputs, 256 hidden nodes in one layer, and 1 output and is being trained on 10,000 randomly chosen molecules for 200 iterations at a learning rate of 0.01. This ANN is performing much better than any of our previous ANNs, further supporting our hypothesis that the 256-bit feature vectors were missing a lot of information. The internal RMSE is 0.12031. Scoring our new neural network on 10,000 other random rows gives a RMSE of 0.1535, which is much nicer than the 0.28 we were scoring with our other models. The takeaway here is that feature engineering is very important: the better we can represent our data, the better our results will be. We verified this takeaway by running our random forest regressor on a 1024-bit vector. Using 50 trees, training on 70% of the data and testing on the remaining 30%, we were able to achieve RMSE 0.115461. Finally, we are running the neural network using thees same features (with 1024 inputs, 512 hidden nodes, and 1 output) overnight. The neural network with 512-bit vectors seemed to have a good balance between underfitting and overfitting, as well as efficiency on our machines. Given enough time, we suspect we can get the error very low by retraining the neural network for a long time.

5 References and Citations

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