

Practical 1: Regression

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1 Technical Approach

We began by performing exploratory analysis on the sample dataset we were given, which consisted of a training set of 1 million molecules with 256 binary predictors, in addition to their SMILES string and the HOMO–LUMO gap we were seeking to predict. The test set consisted of 824,230 molecules with the same set of predictors as well as their SMILES string. The sample code we were given implemented a default Linear Regression model on the full set of 256 predictors, yielding an $R^2_{\text{LR}} = 0.461$ ($\text{MSE}_{\text{LR}} = ?$) over the full training set, and a default Random Forest regression with $R^2_{\text{RF}} = 0.554$ ($\text{MSE}_{\text{RF}} = ?$).

Initial inspection found that out of 256 molecular features, 221 of them were unexpressed (i.e. had $x_i = 0$) for *all* molecules, both in the training set and the test set. Dropping unimportant features would normally call for K -fold cross-validation across the training set to ensure those features are consistently unimportant in all cases. However, in the case of null values of certain features for every element of the training set, it is not only legitimate but necessary to drop those features from all further analysis, as fitting along null dimensions would constitute a form of overfitting.

Having reduced the sample dataset to 31 expressed molecular features, we performed both regularized and non-regularized linear regression with cross-validation¹ and hyperparameter tuning, under the following methods:

1. Non-regularized linear regression: Yields $R^2 = \dots$
2. Ridge Regression:
3. Lasso:
4. Elastic Net:

The results from linear regression on the sample dataset consistently gave us low predictive value, even when compared to generic random forest regression, which led us into pursuing 2 parallel tracks:

¹After initially trying 3-fold, 5-fold and 10-fold cross-validation, we settled on 5-fold cross-validation as the best compromise between accuracy and computational speed.

1. Feature engineering: (*Fangli*)
2. Non-linear methods: (*Xihan, Antonio*)

Among these we concentrated on 2 broad categories:

- (a) Tree based methods / Ensemble methods (*Xihan*)
- (b) Deep learning: Since the predictors describe a broad set of molecular properties, it is natural to expect non-linear interactions between them to play a role in determining the HOMO-LUMO gap. For this reason we decided to explore the training of simple neural networks that would serve to model these interactions and got acquainted with the basics of Deep Learning as a tool to tackle this problem. In all cases, we used an architecture of one or more dense (fully-connected) hidden layers between the input layer of N parameters and the output layer of 1 node for the response we wanted to model. For each node in the hidden layers, we used the widely used “relu” function ($f(x \leq 0) = 0, f(x > 0) = x$) as activation function. We trained the model using the *keras* module in Python, using the *adam* optimizer for the learning rate, and setting aside 20% of training data for validation. The model would be fitting for the weights of the connections between pairs of nodes in the network, which in the case of 1 hidden layer with M nodes, would result in $(N + 1) \times M$ parameters to be trained.

Taking a trial-and-error approach to setting the network architecture, we show the results of validation set MSE for 3 broad cases, using the 31 expressed features in the sample training dataset: 1) 1 hidden layer with variable number of nodes, 2) 2 hidden layers, with 31 nodes on the first and variable number of nodes on the second, and 3) 3 hidden layers, with 31 nodes on each of the first two, and variable number of nodes on the third.

Figure with 3 plots for 1, 2 and 3 hidden layers

The result of this experiment showed that the MSE was not as sensitive to the addition of a second and third layer, as it was to the number of nodes in the first layer of the 1-hidden layer architecture. Given the computational limitations that were expected for a much larger set of features, we used this result to use the feature-engineered set to train only 1-layer models with a limited number of nodes in the same range as the number of predictors.

How did you tackle the problem? Credit will be given for:

- *Diving deeply into a method (rather than just trying off-the-shelf tools with default settings). This can mean providing mathematical descriptions or pseudo-code.*
- *Making tuning and configuration decisions using thoughtful experimentation. This can mean carefully describing features added or hyperparameters tuned.*
- *Exploring several methods. This can contrasting two approaches or perhaps going beyond those we discussed in class.*

Thoughtfully iterating on approaches is key. If you used existing packages or referred to papers or blogs for ideas, you should cite these in your report.

Mention Features	
Feature	Value Set
Mention Head	\mathcal{V}
Mention First Word	\mathcal{V}
Mention Last Word	\mathcal{V}
Word Preceding Mention	\mathcal{V}
Word Following Mention	\mathcal{V}
# Words in Mention	$\{1, 2, \dots\}$
Mention Type	\mathcal{T}

Table 1: Feature lists are a good way of illustrating problem specific tuning.

Model	Acc.
BASELINE 1	0.45
BASELINE 2	2.59
MODEL 1	10.59
MODEL 2	13.42
MODEL 3	7.49

Table 2: Result tables can compactly illustrate absolute performance, but a plot may be more effective at illustrating a trend.

2 Results

This section should report on the following questions:

- Did you create and submit a set of predictions?
- Did your methods give reasonable performance?

You must have *at least one plot or table* that details the performances of different methods tried. Credit will be given for quantitatively reporting (with clearly labeled and captioned figures and/or tables) on the performance of the methods you tried compared to your baselines.

3 Discussion

End your report by discussing the thought process behind your analysis. This section does not need to be as technical as the others but should summarize why you took the approach that you did. Credit will be given for:

- Explaining the your reasoning for why you sequentially chose to try the approaches you did (i.e. what was it about your initial approach that made you try the next change?).
- Explaining the results. Did the adaptations you tried improve the results? Why or why not? Did you do additional tests to determine if your reasoning was correct?