Task2WriteUp

2024-12-09

Task 2: Feature Selection

Abstract Task 2

The focus of the following analysis is to attempt to achieve high classification accuracy, while using a minimal number of features on very highly dimensional data. We will use a combination of six different feature selection and classification techniques to accomplish the goal. The models and methods used are a combination of methods taught in our ST443 Machine Learning and Data Mining Course taught at the London School of Economics and Political Sciences, and other techniques used from personal research.

Data Description

We were given one dataset that contains binary features that describe the three-dimensional properties of a molecule in a compound or a random probe across different compounds. The data contains 800 observations, which represent 800 compounds, and 100,000 columns (50,000 real variables and 50,000 random probes). The first column named *label* represents whether a compound bound to a target site on thrombin[1].

Exploratory Data Analysis

Most of our exploratory data analysis was undertaken with the goal of preliminary feature reduction prior to model implementation. After confirming that there were no missing values within our data, we aim to remove features with extremely low to zero variance. The following histograms depict the number of compounds found to have bound to a particular target site and the associated variance . . .

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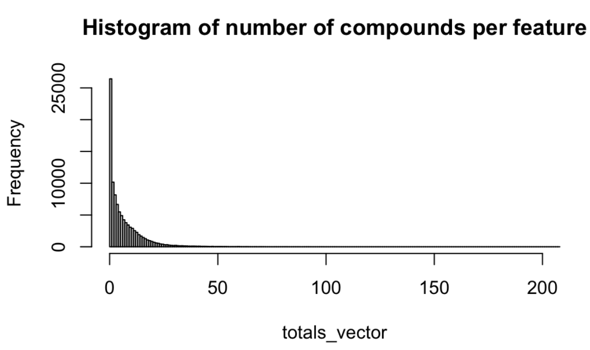
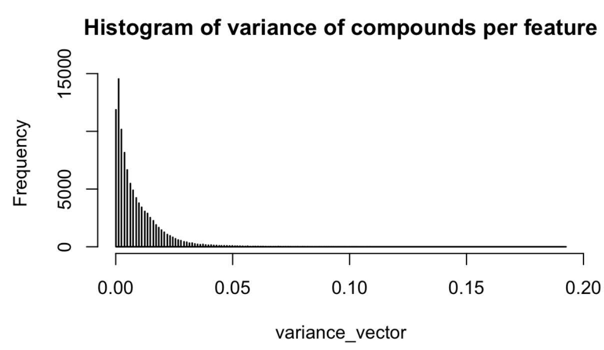




[1]Thrombin is an enzyme that plays a key role in blood clotting and other biological processes.

Models

Lasso The first model we attempted to run was logistic classifier with a Lasso-Penalty term. The lasso penalty term is a common regularization technique used for feature selection as it shrinks some of the coefficient estimates to be exactly equal to zero, effectively removing them from the model. The ability to shrink coefficients to zero depends on the magnitude of the tuning parameter, lambda (λ), which we tune in our model. The best way to choose an optimal λ is through cross validation, which we apply in our models. For our data, we believed that the lasso coefficient will be most meaningful on a logistic classifier, this is because our predicted variable is binary which takes values of either 1 or -1 (we convert -1 to 0 for simpler interpretation of probabilities). In our approach, we use a five-fold cross validation, with a grid of 100 different values of λ. We also use weights to account for the highly imbalanced data. For each λ, we calculate the predicted probability where we then decide to classify anything with a probability of 0.5 or more to the "*1*" class else, the "*0*" class. Then using those predictions we calculate the balanced accuracy, and count the number of selected features for each lambda. Since we want to account for best balanced accuracy, and lowest amount of features, we use a scoring formula where *score = balanced accuracy - 0.001***(number of features)*. This way we penalize results that have too many features. We then extract the lambda with the best score, train the data again using that lambda, then test the model using our test data and report the number of features selected. The table below shows different results for different predictors including the model with the worst score, worst balanced accuracy on the cross-validation, the best score:

Model	Lambda Value	Number of Selected Features	Balanced Accuracy
Worst Score	1e-04	234	0.8189
Best Score	0.0475081	47	0.8189
Worst BA	0.2719	1	0.8189

Forward Stepwise Selection (FSS)

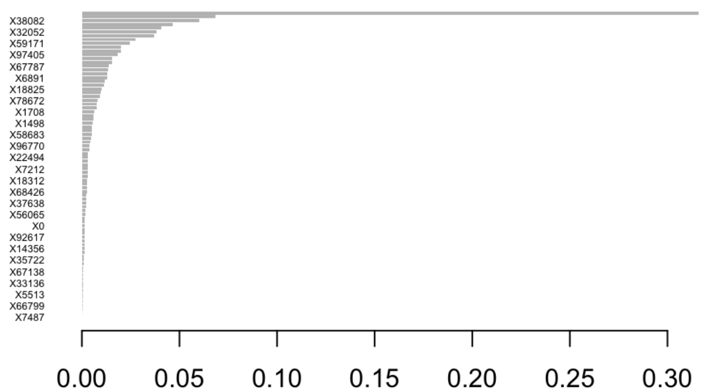
Random Forest

Elastic Net After the results obtained from the logistic classification method with a lasso penalty term, we thought that it could be interesting to compare with the results of an elastic net. An elastic net is another regularization technique which combines both the Lasso (L1) and the Ridge (L2)[2] penalties.Since the elastic net penalty is not as harsh as the Lasso penalty, we assumed it will return more features, but we were interested in seeing if the elastic net could improve the balanced accuracy. The elastic net penalty depends on two main parameters, λ, (the strength of the penalty term) and α (the mix between Lasso and Ridge). We use a process very similar to the one used for the Lasso penalty term on the logistic regression, only we also try different values of α. The table below shows results for the best scores, worst scores, and worst balanced accuracy on the validation set:

Model	Alpha Value	Lambda Value	Number of Selected Features	Balanced Accuracy
Worst Score	0.4	0.1205	101	0.8257
Best Score	0.49	0.0955	88	0.8608
Worst BA (cv)	0.46	0.1205	75	0.8608

[2]The Ridge Regularization technique is one that shrinks the coefficients on the predictors, but never to 0, so it keeps all coefficients in a model.

XGBoost Boosting is another technique that can be relevant for feature selection. Boosting combines weak learners (usually decision trees) to create a strong learner, and it does so by building models sequentially and attempting to correct the errors made n the previous model. While boosting, the algorithm records the importance of each feature based on how much it improved the model's performance. A boosting algorithm stores an importance score for each feature, and that way some features can be dropped. We attempted to use the XGBoost (Extreme Gradient Boosting) algorithm. XGBoost, is a boosting algorithm that is able to handle very large datasets and uses regularization techniques as well. Since XGBoost handles imbalanced data quite well, we decided to not weight the data. Our process is similar to the one used for Lasso and the Elastic net, where we loop over certain hyper parameters, most importantly λ, which represents the shrinkage parameters, specifically the rate which boosting learns. We then returned the model which returned the best balanced accuracy on the cross validation, and then used that model to make predictions on the test data. The number of features selected were extracted from the XGB importance matrix, which calculates importance based on gain, cover and frequency.[3].Features with 0, are excluded from the matrix. Below is a chart for the features selected for our best XGBoost Model. We found that the best learning rate, λ, was equal to 0.5!



Support Vector Machines (SVM)

Results

Model	Num. of Features	Bal. Accuracy	Accuracy	F1
Logistic Lasso	47	0.8189	0.925	0.6
FSS	208	0.7805	0.9188	0.5517
Random Forest	100	0.8223	0.9313	0.6207
Log. Elastic Net	88	**0.8608**	**0.9375**	**0.6667**
XGBoost	81	0.8257	**0.9375**	0.6429
SVM (Linear Kernel)	**35**	0.8574	0.9313	0.6452

[3]Gain is the improvement in accuracy brought by a feature to the branches it is on. Cover represents the second derivative to the loss function with respect to a variable, a large value means the feature has a large importance on the loss function. Frequency represents the number of times a feature is used in all generated trees.

Conclusion

The results above, show us that there is an inherent trade-off between the number of features, and the evaluation metrics such as the balanced accuracy on the test data. The reason we care about taking into consideration the smaller amount of number of features has to do with both efficiency and interpretability. For example, if one were to conduct future research, they could focus on a smaller subset of features.

Depending on one's preferences and goals, either the Elastic Net or the SVM model seem to be good models for the classification for whether a compound will bind to a target site.

Strengths and Weaknesses Our first attempt at running many of our models, we encountered computational/memory limit-issues. To combat this, we had to aggressively reduce the dimensionality of our data before feature selection from our models could take place. We subset the data based off of features' variance, removing features with less than 0.01 variance. Ideally we would have been able to run the entire original data (100,000 features) through the models and allow them to *naturally* select the relevant features.

Another difficulty we encountered, was the imbalance of the data. The original dataset had less than 10% of observations that were labeled by the positive class. This could have led to bias in the model towards the more frequently-observed negative class. Measures such as accuracy might be mislead by this bias, and we therefore we used balanced accuracy to evaluate our models instead.

The strength in our approach is that we employ many different types of feature selection methods. Each one attempts to identify the most important features in different manners.

Future Research A main goal of future research could be to improve the methods listed above in the hopes of obtaining even stronger results, there are multiple ways we can do this. 1.Ideally, our data would include more compounds (observations) so that there would be more even dimensionality, which would better protect our models from overfitting! 2. More time, computational power, and lower dimensional data would allow better tuning of the parameters. 3. We could identify features that are highly multicollinear. Failing to remove them,could lead to instability and inefficiency in our models.

Refrences

Guyon, I., Gunn, S., Ben-Hur, A. and Dror, G. (2004) Result Analysis of the NIPS 2003 Feature Selection Challenge. In Advances in Neural Information Processing Systems (Saul, L., Weiss, Y. and Bottou, L., eds.), vol. 17, MIT Press.

Shlobin NA, Har-Even M, Itsekson-Hayosh Z, Harnof S, Pick CG. Role of Thrombin in Central Nervous System Injury and Disease. Biomolecules. 2021 Apr 12;11(4):562. doi: 10.3390/biom11040562. PMID: 33921354; PMCID: PMC8070021.