

Classifying New Particle Formation

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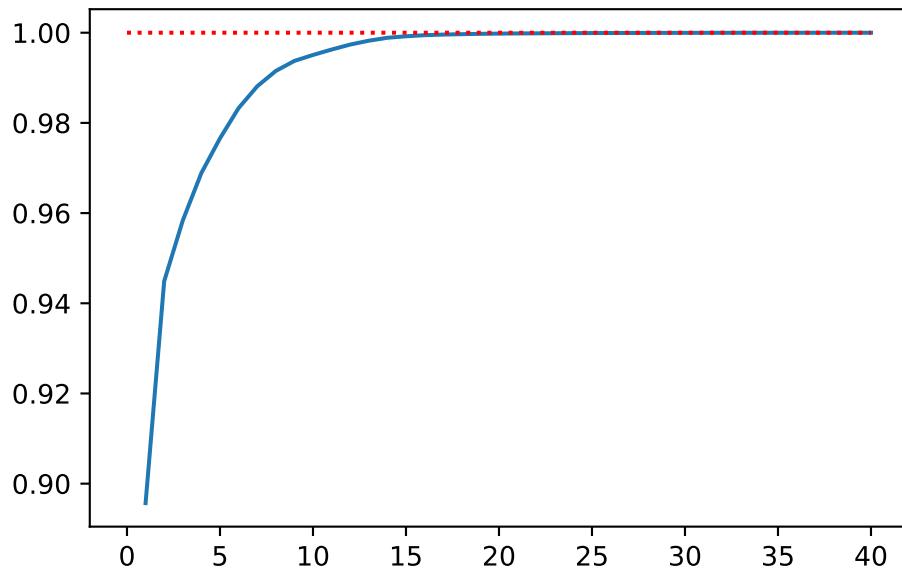
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Preprocessing

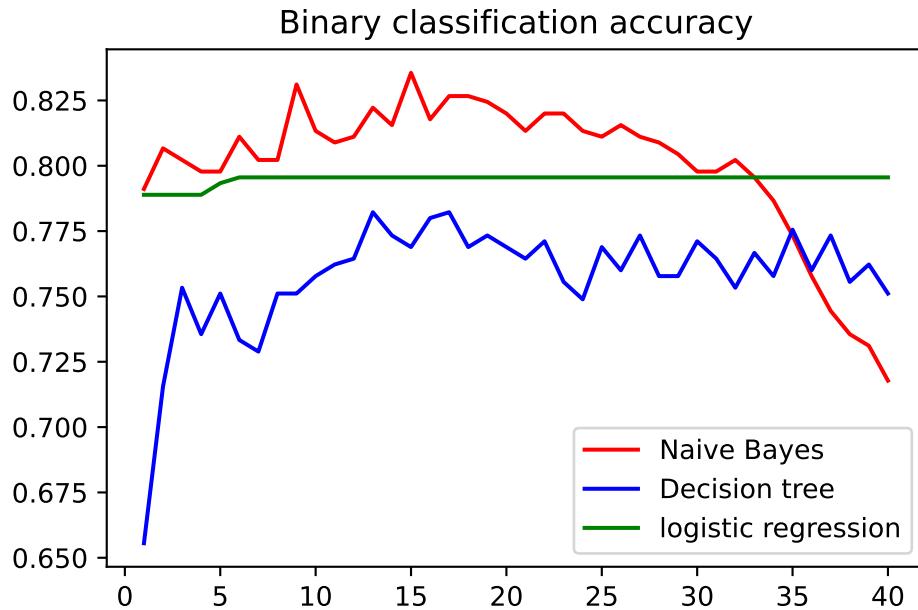
We decided to start by trying feature selection and dimensionality reduction via principal component analysis with a few different machine learning models.

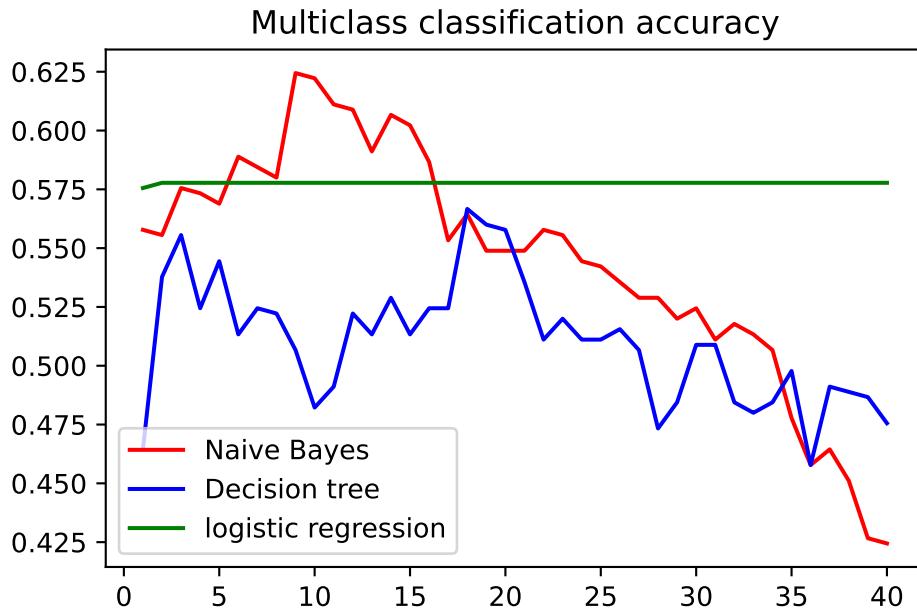
Principal component analysis

First we looked at cumulative proportion of variance explained by the principal components. We used l2 normalization. We looked at the behaviour of PCA and all the models at upto 100 components, but nothing interesting happened with any of them beyond about 40 components, so the charts here focus on 40 or less components. Accuracy is measured as the average accuracy using 10-fold cross validation.



Then we looked at the accuracy of logistic regression, decision tree and gaussian naive Bayes classifiers with different numbers of principal components for binary and multiclass classification.





The gaussian Naive Bayes classifier with 9 predictors is clearly the best overall performer out of the tested models.

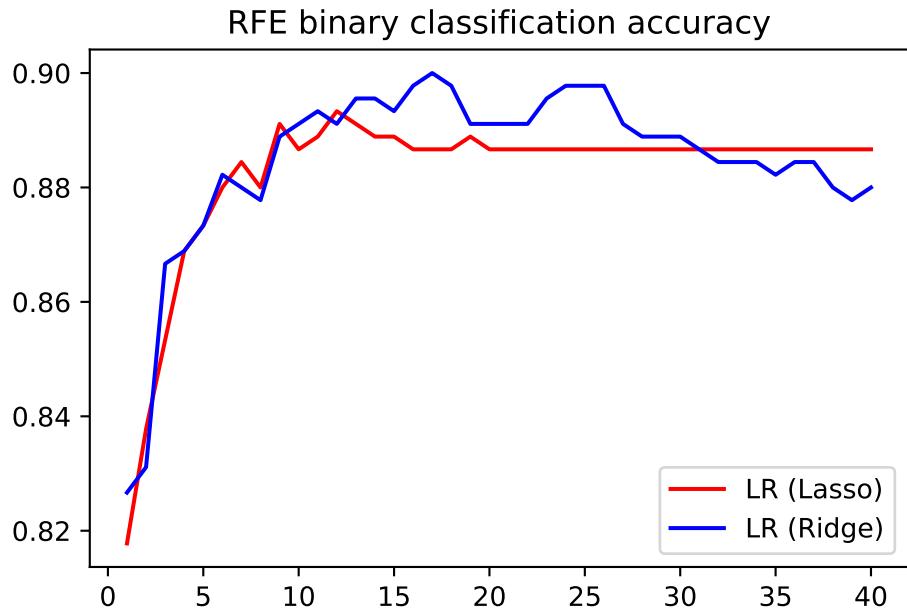
Feature selection

Another preprocessing method is feature selection, for which we have used Recursive Feature elimination using 5-fold cross validation, which is a form of backward selection. With RFE we get the following results for binary classification

Model	Optimal n of features	Best accuracy	Accuracy without RFE
0 LR L1	12	0.891111	0.886667
1 LR L2	17	0.897778	0.875556

on this table we can compare the improvements RFE provides, able to increase binary classification accuracy by couple percent compared to including all features.

Note: I was using liblinear LR model which cannot do multiclass classification. fix is todo. also could add more models



We can see that increasing features results in better accuracy, usually having the best accuracy at 10-20 features. We currently only have linear regression with L1 (lasso) and L2 (ridge) penalties. After comparing different models, we will probably use some combination of PCA and Feature selection in our final model