

# Classifying New Particle Formation

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Increase the number of iterations to improve the convergence (max\_iter=100).

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Please also refer to the documentation for alternative solver options:

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```

Group: John 117

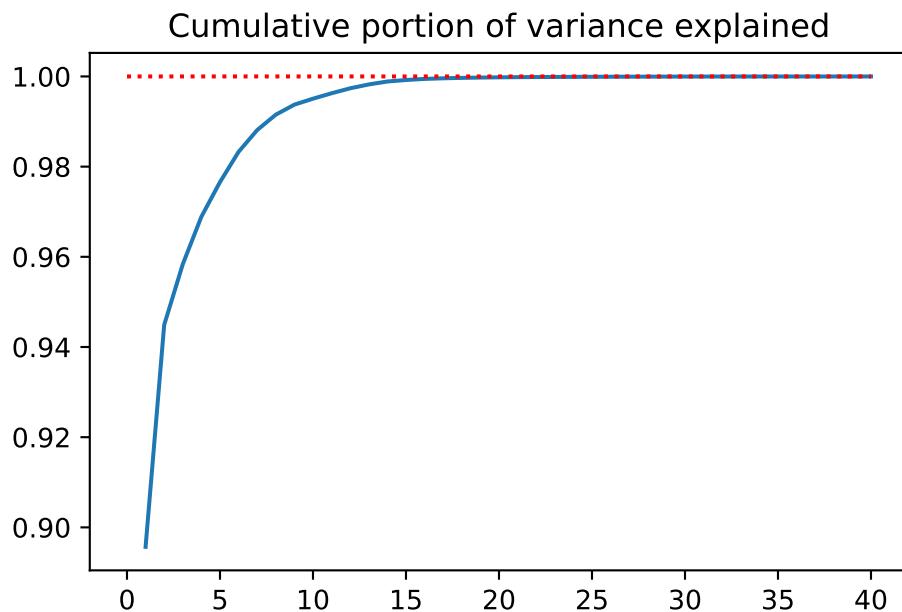
Members: Elias Toukolehto and Joacim Sarén

## Preprocessing

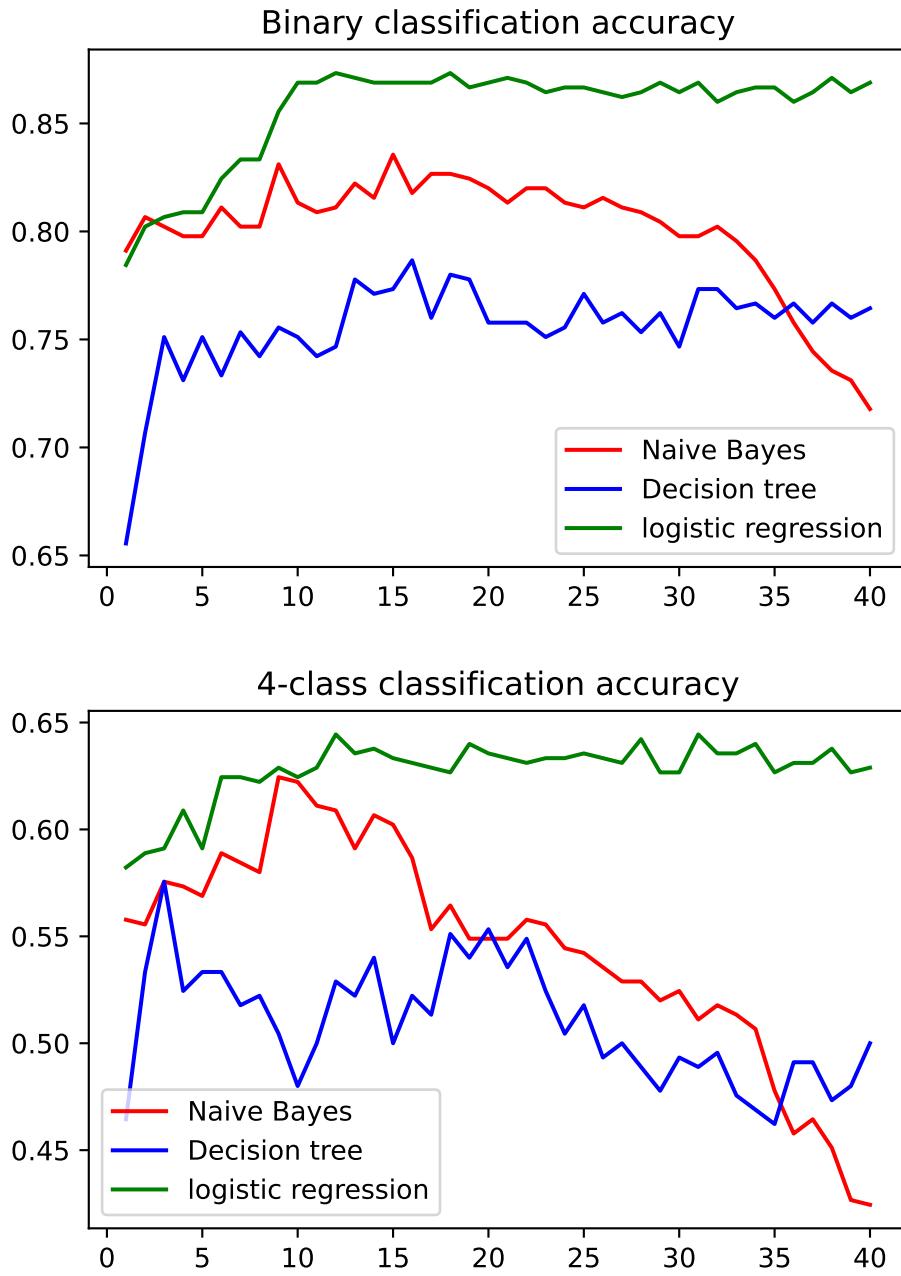
We decided to start by trying feature selection and dimensionality reduction via principal component analysis with a few different machine learning models.

### Principal component analysis

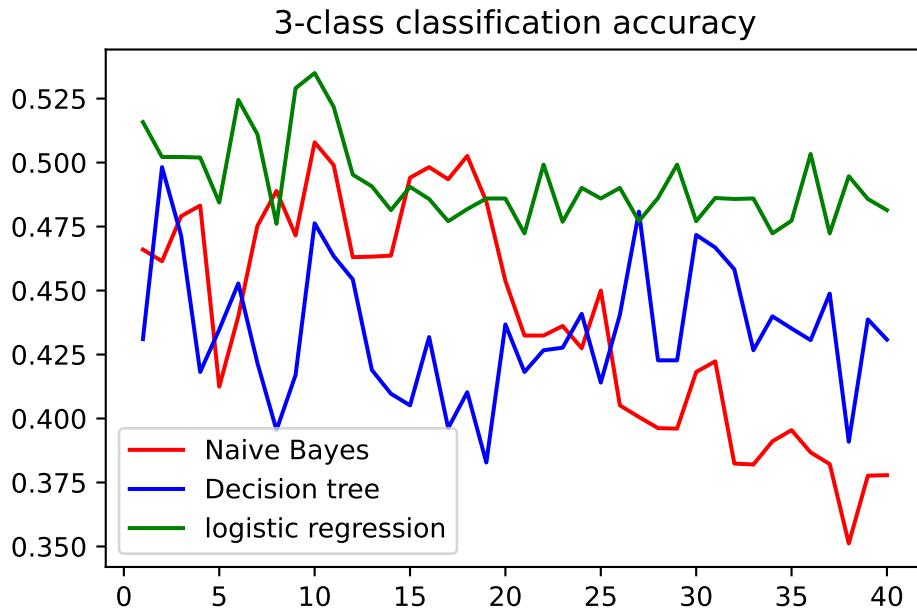
First we looked at cumulative proportion of variance explained by the principal components. We decided to use PCA for it's relative simplicity. We used l2 normalization in order to keep all predictors in consideration when running PCA. We looked at the behaviour of PCA and all the models up to 100 components. We won't show data beyond 40 components, because it didn't show any interesting behaviour that's not visible with lower values. This is mainly to keep the charts more readable.



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 4-class classification using 10-fold cross validation.



The gaussian Naive Bayes classifier with 9 predictors is clearly the best overall performer out of the tested models. Because the task focuses on binary classification, which is also easier, we wanted to explore a 2-tier classifier. First tier separates events and non-events, and the 2nd classifies events to the specific event classes. To choose the model for the 2nd tier, we looked at the 3-class classification accuracy of the same classification methods trained on data only containing events.

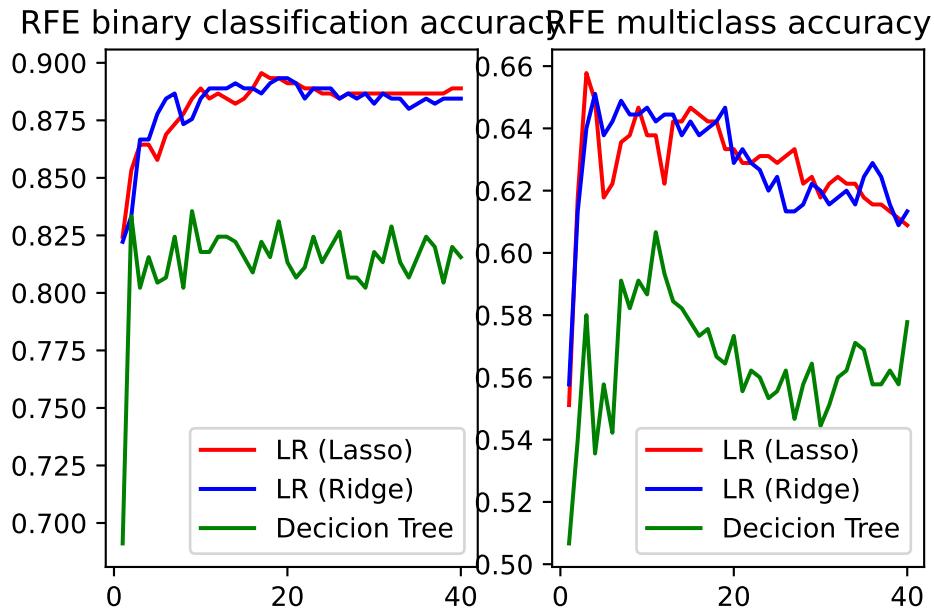


## Feature selection

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	17	0.893333	0.891111
1	LR L2	19	0.893333	0.886667
2	DT	9	0.817778	0.811111
	Model	Optimal n of features	Best accuracy	Accuracy without RFE
0	LR L1	3	0.648889	0.626667
1	LR L2	4	0.637778	0.613333
2	DT	11	0.593333	0.571111

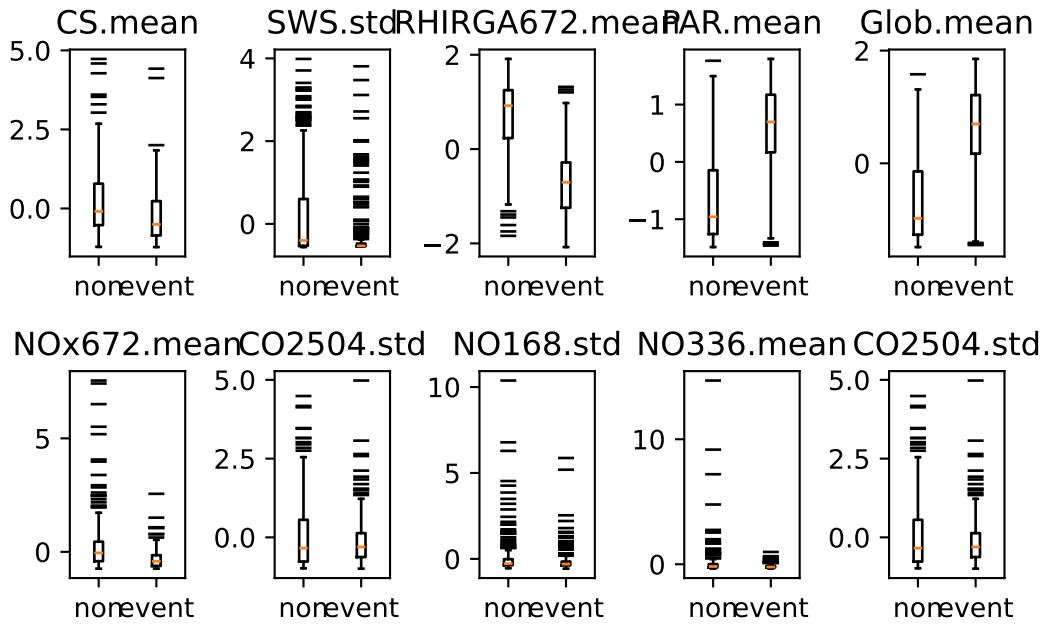
on this table we can compare the improvements RFE provides, able to increase binary classification accuracy by couple percent compared to including all features.



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

## Feature analysis

Analyzing coefficients allowed us to rank some features by usefulness. The ones for the plot below were defined by performance with logistic regression using 5-fold cross validation.



Here are boxplots of some of the most useful (top row), and least useful (bottom row) features for binary classification in the dataset. For the reliable features we can see that the quartile ranges don't have much overlap, as for the unreliable features there is a lot of overlap between classes. CS.mean is an outlier, where models find it very useful even though it has surprisingly similar boxplots between classes.