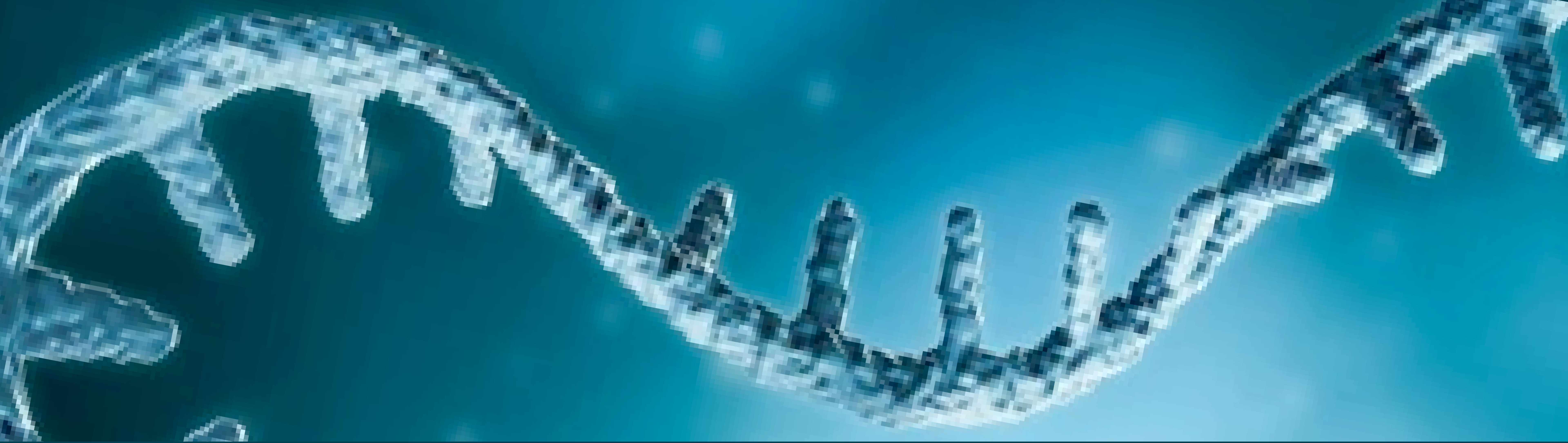
shutterstock.com 1907619613 royalty free

Cancer Gene Expression Classification

https://github.com/tamarahorne/Springboard/tree/main/Capstone%20Project%203

Tamara Horne | May 2023| Springboard—DSC Capstone Project 3



Introduction

The Value of Predicting Cancer Type from Gene Expression Data

Tamara Horne
2023 | May

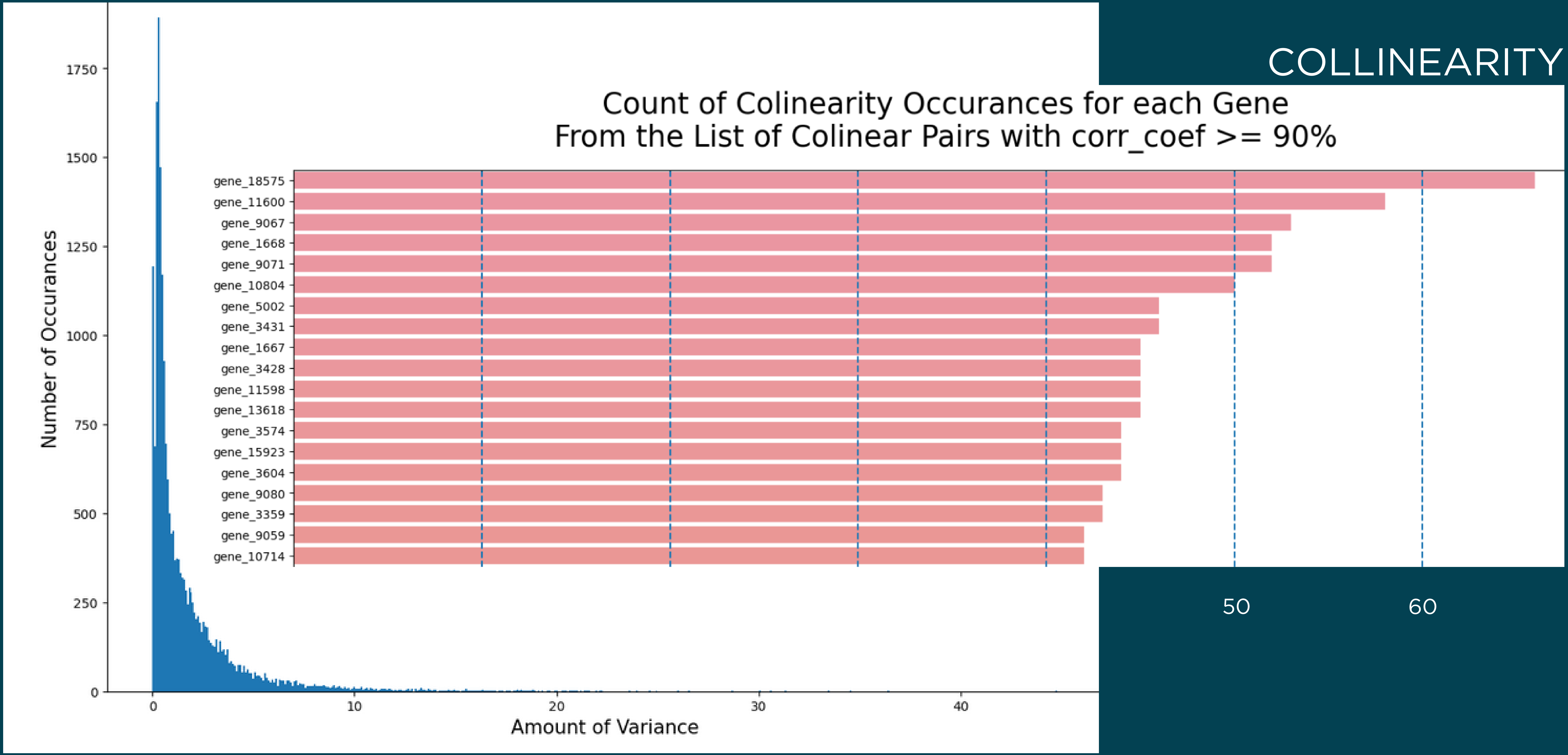
THE DATA

- subset of the RNA-Seq (HiSeq) PANCAN data set
- samples from five cancer types
    - BRCA (breast)
    - KIRC (kidney)
    - COAD (colon)
    - LUAD (lung)
    - PRAD (prostate)
- 801 rows; 20531 columns
- one row represents one sample
- one column contains a value for the gene expression for one gene
- columns have dummy names (gene_XX)
- no missing values

Concerns

VARIANCE DISTRIBUTION

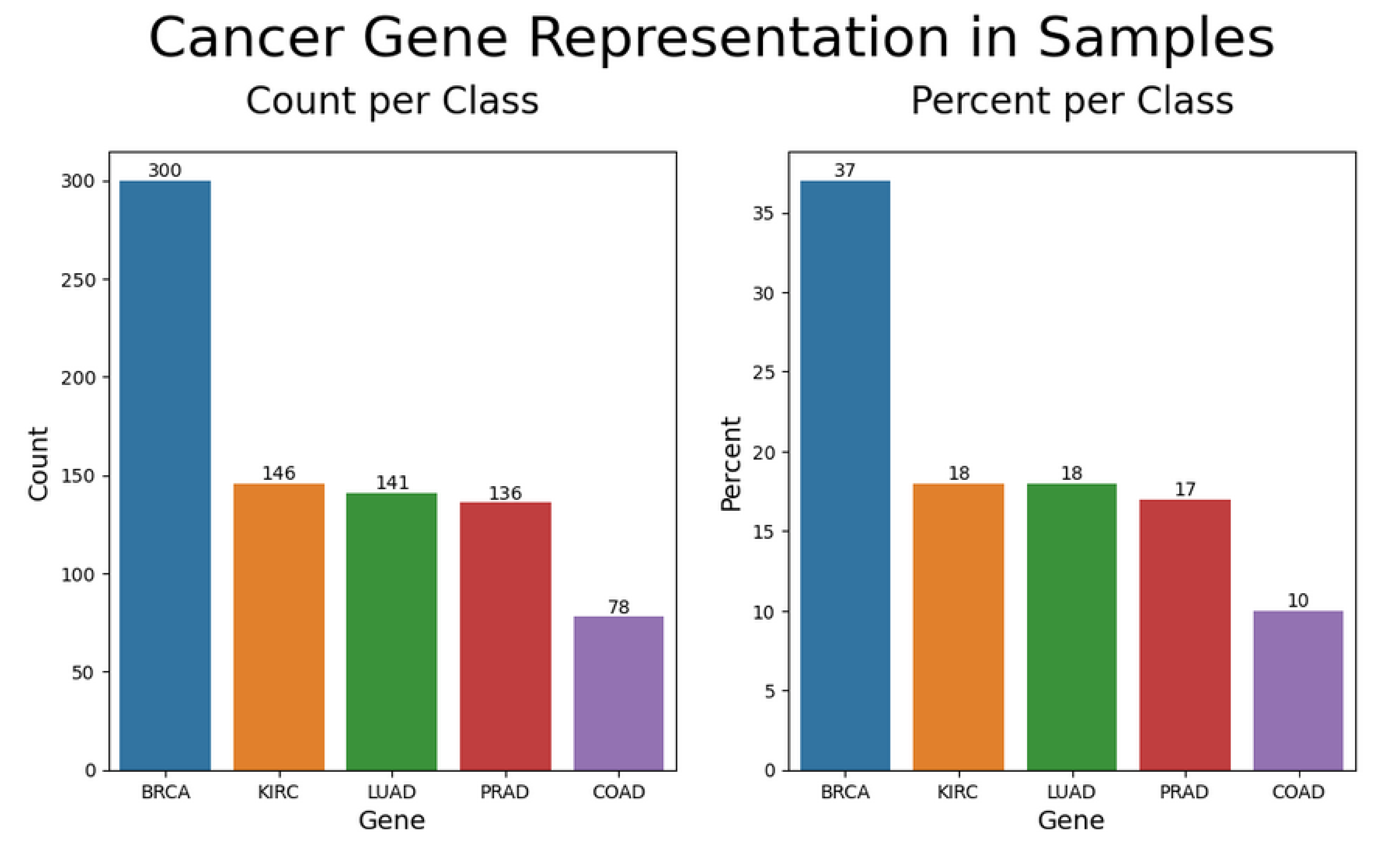
COLLINEARITY



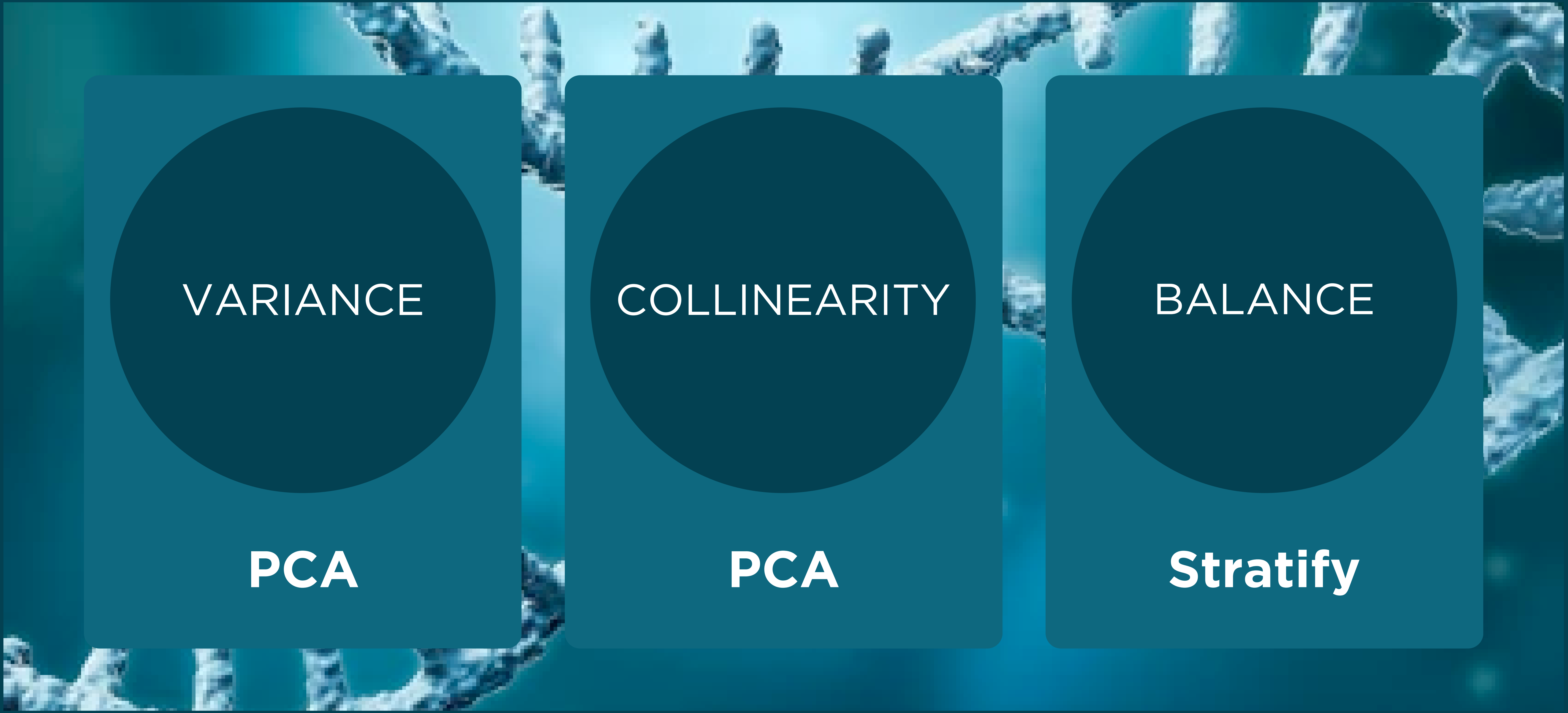
Count of Colinearity Occurances for each Gene
From the List of Colinear Pairs with corr_coef >= 90%

Concerns

BALANCE



Decisions



VARIANCE

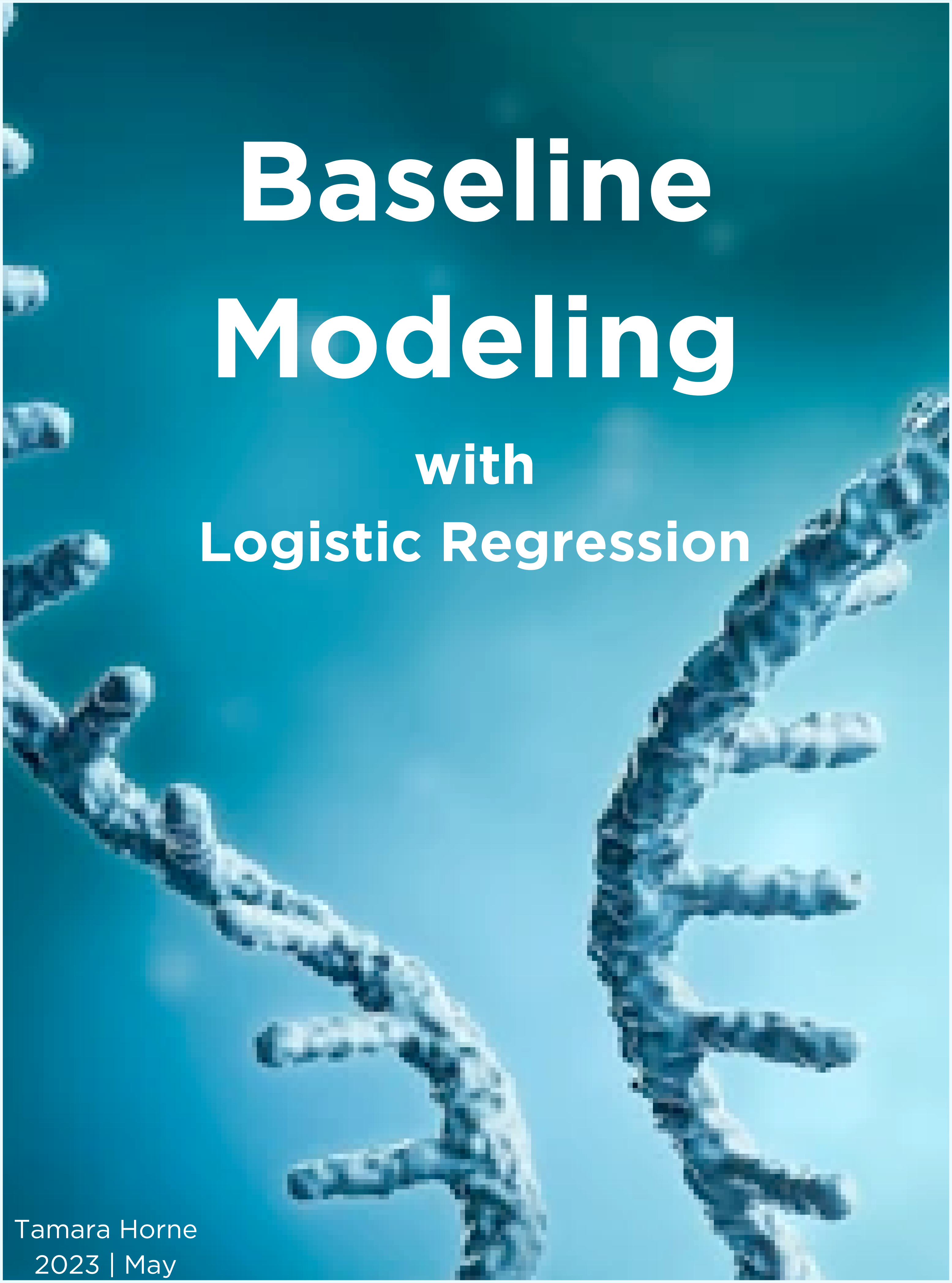
PCA

COLLINEARITY

PCA

BALANCE

Stratify



Baseline Modeling

with

Logistic Regression

Tamara Horne
2023 | May

First Steps:

Fixing the Landing Dimension (Rule of Thumb)

●●●

Determine if Using a Scaler in the Pipeline with PCA is Wise

●●●

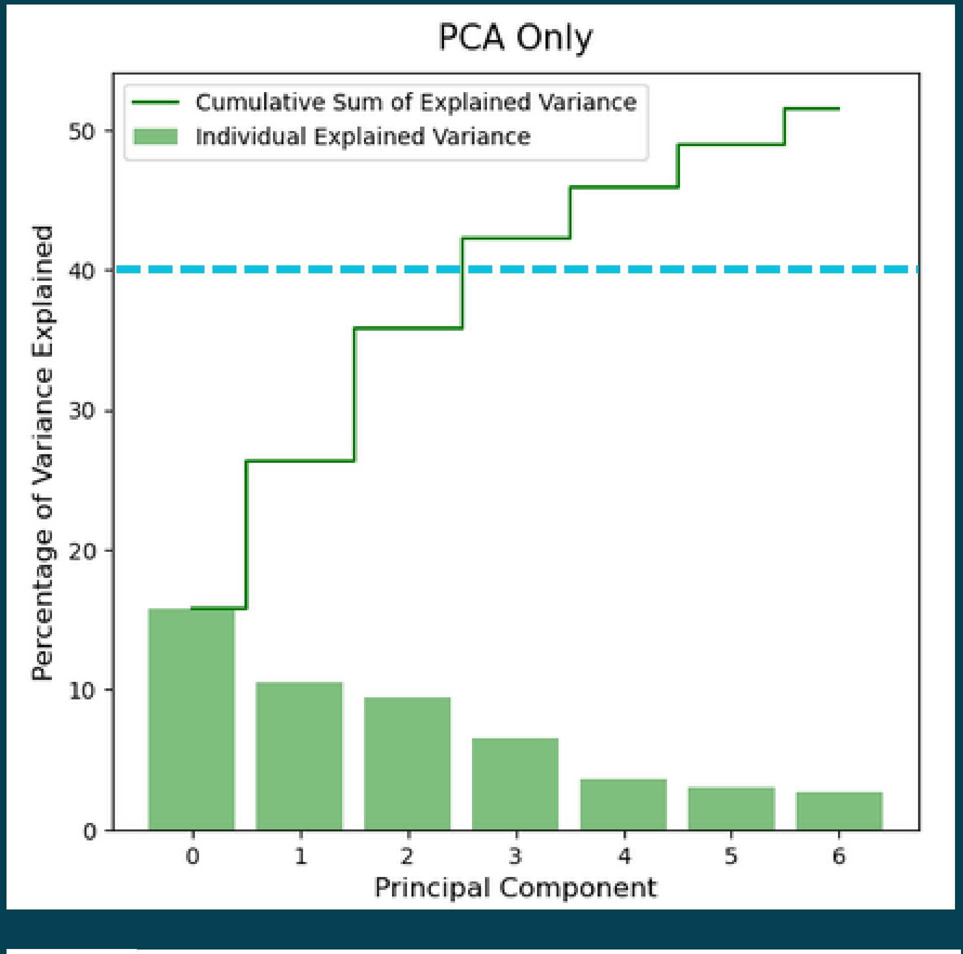
Decide if Balancing of Classes is Needed

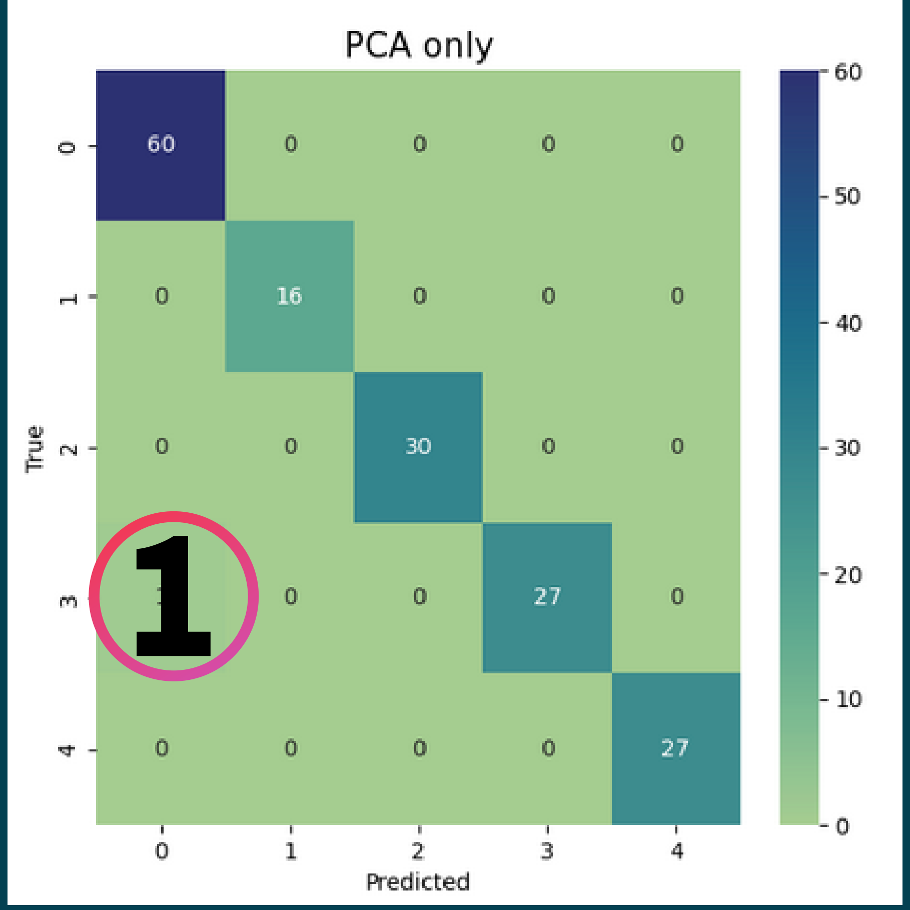
Percentage of Explained Variance

Confusion Matrix

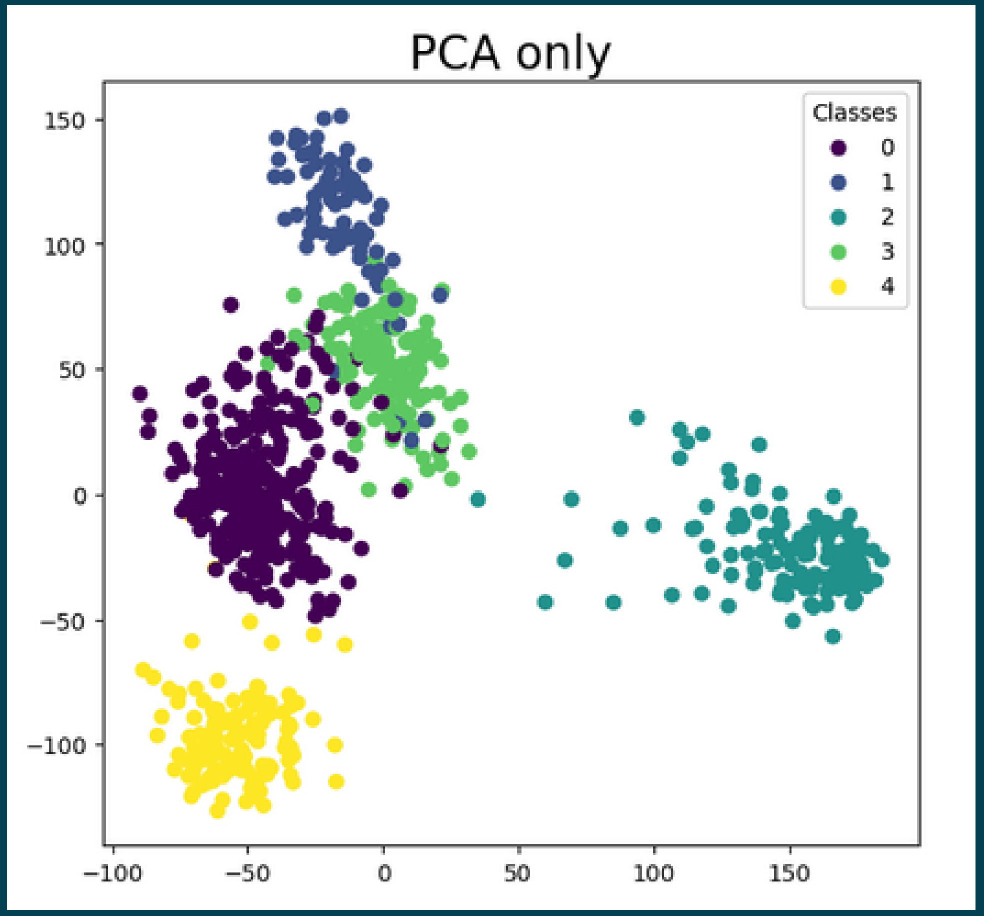
First Two Principal Components

PCA WITHOUT Scaling

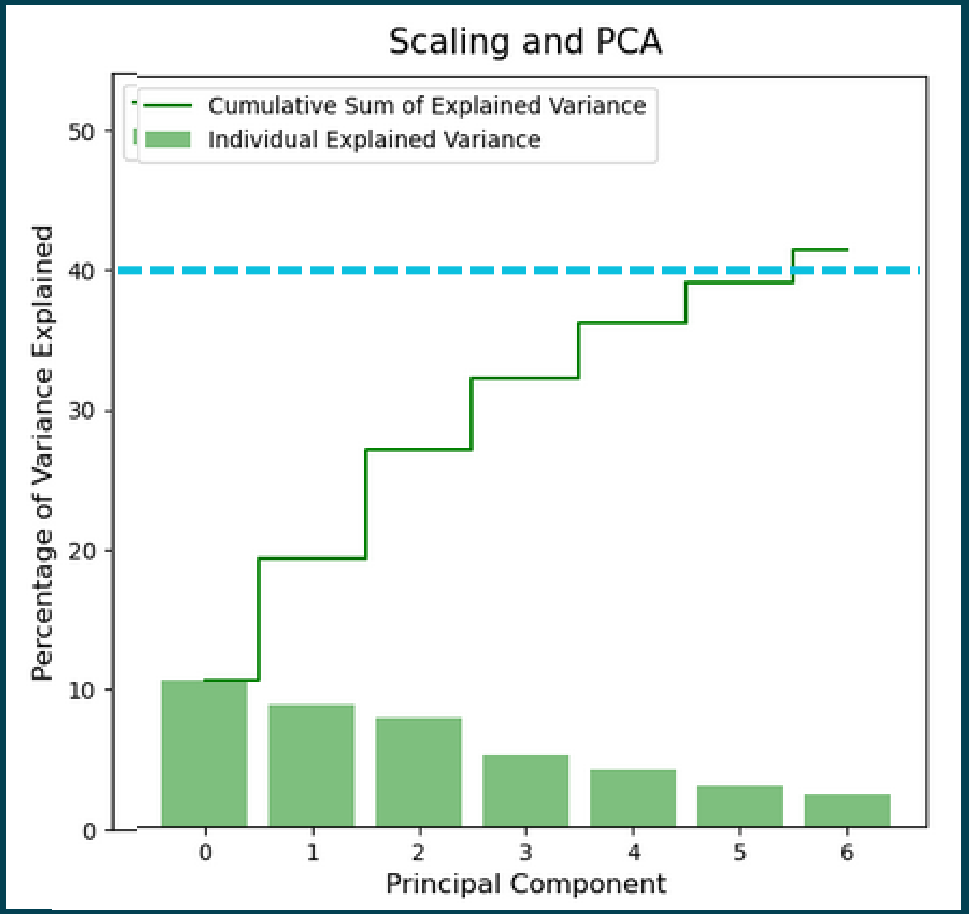


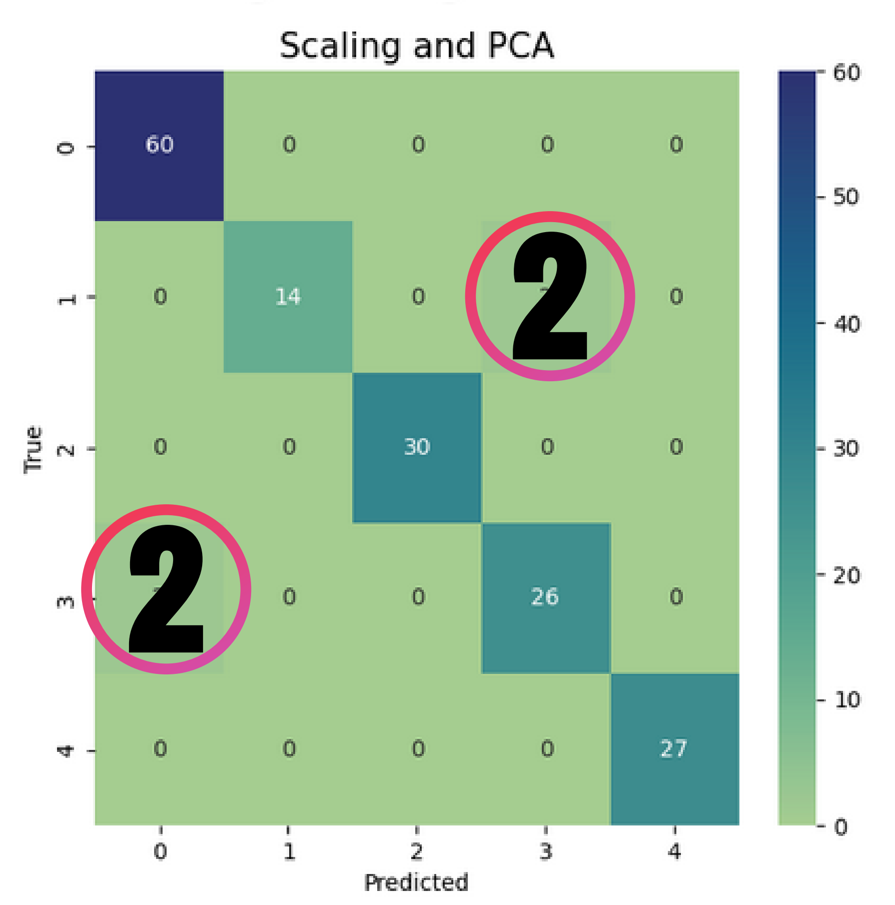

PCA only

True \ Predicted	0	1	2	3	4
0	60	0	0	0	0
1	0	16	0	0	0
2	0	0	30	0	0
3	1	0	0	27	0
4	0	0	0	0	27

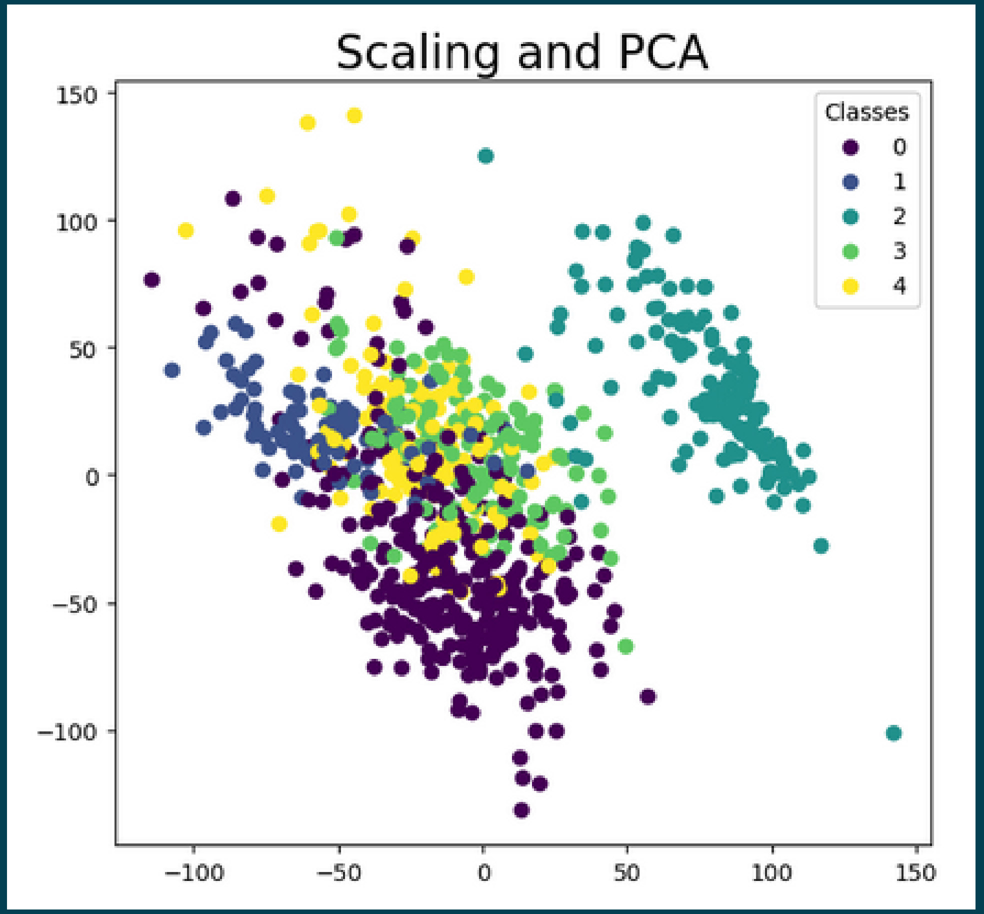


PCA WITH Scaling

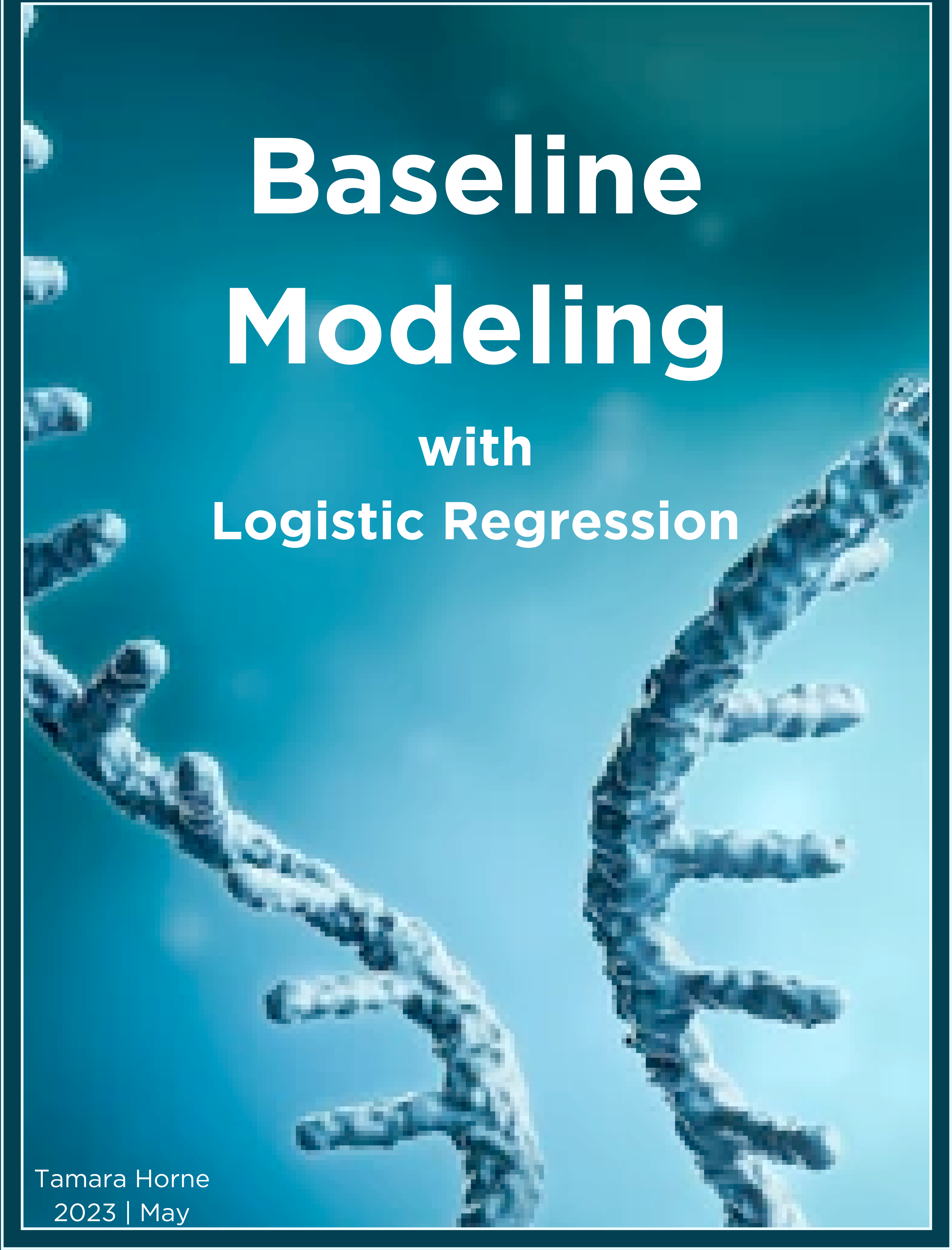



Scaling and PCA

True \ Predicted	0	1	2	3	4
0	60	0	0	0	0
1	0	14	0	2	0
2	0	0	30	0	0
3	2	0	0	26	0
4	0	0	0	0	27



Tamara Horne
2023 | May



Baseline Modeling

with

Logistic Regression

Tamara Horne
2023 | May

Desicions:

Using the Rule of Thumb for Fixing the Landing Dimensions is Sufficient
(Seven Principal Components)

●●●

A Scaler Should Not be Used

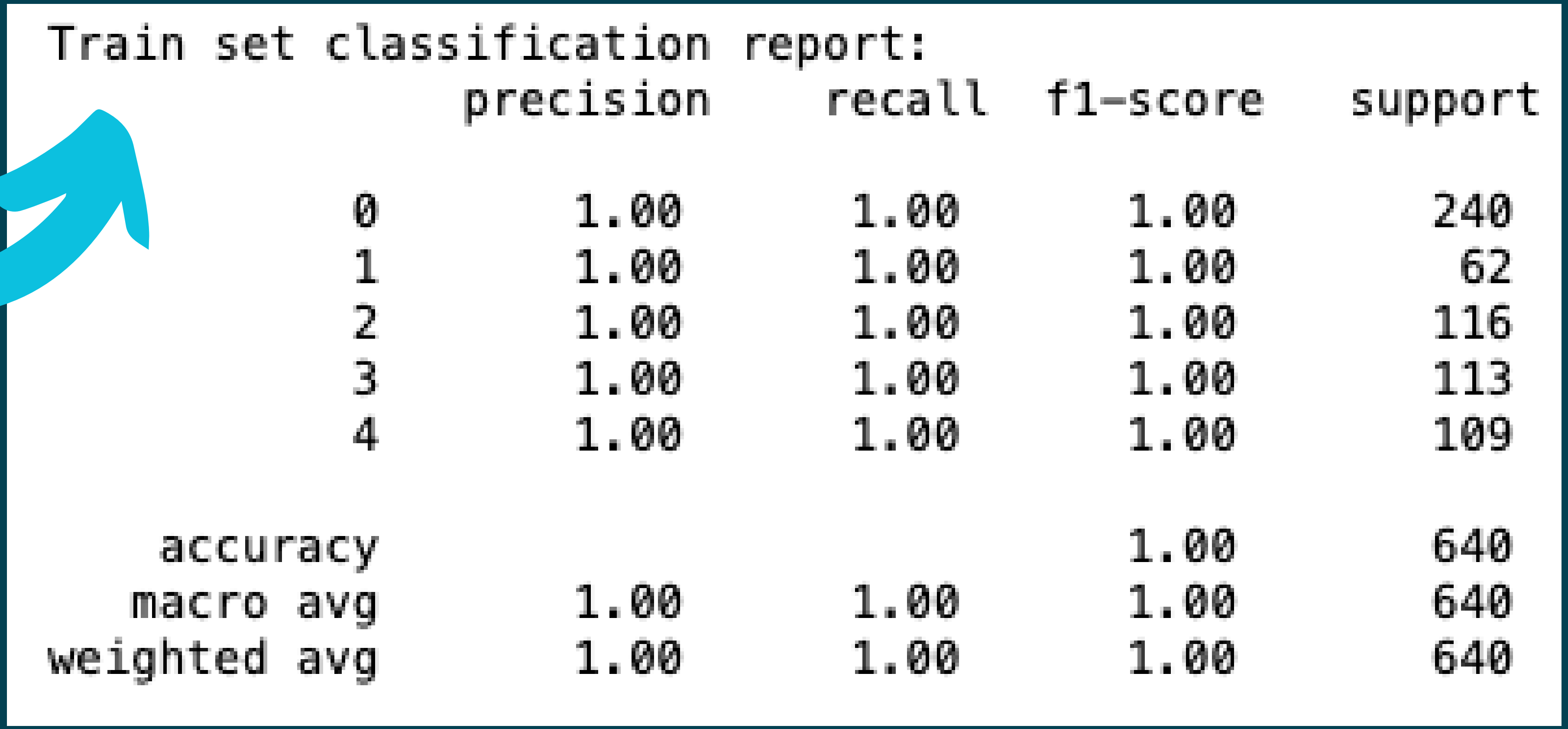
●●●

Balancing of Classes is Not Needed

Baseline Modeling

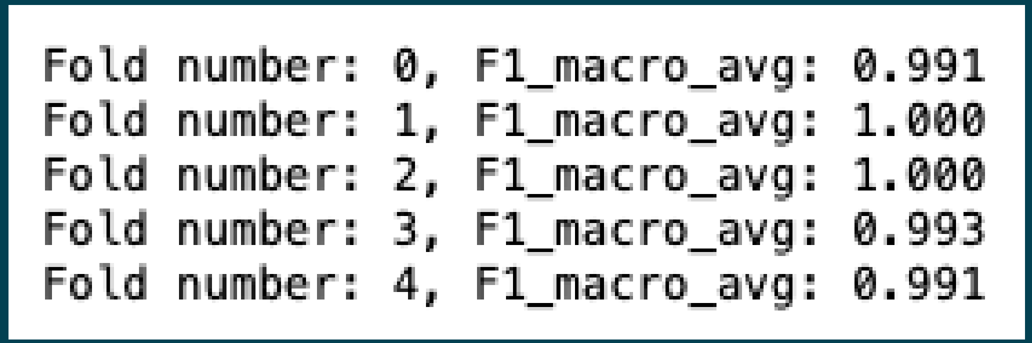
with

Logistic Regression

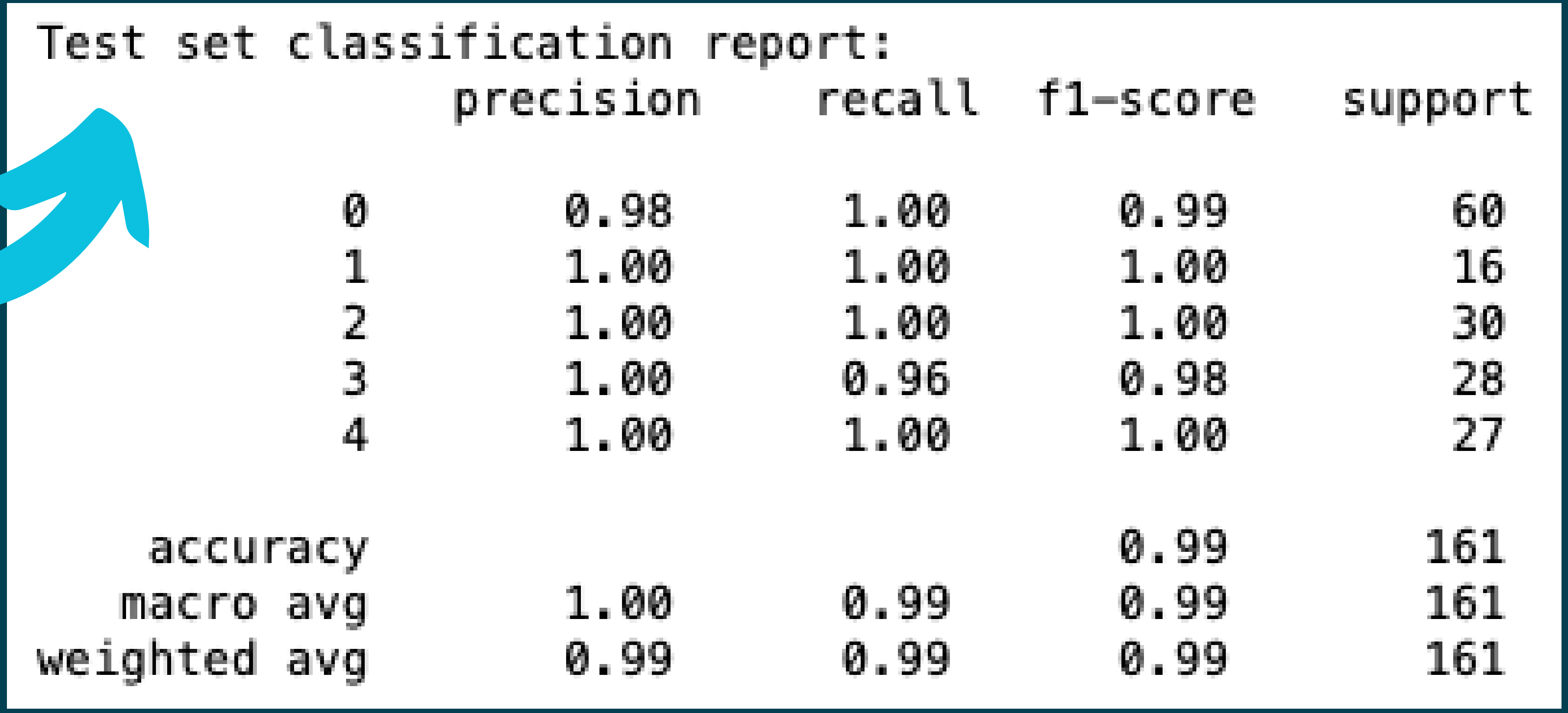


```
Train set classification report:
              precision    recall  f1-score   support

           0       1.00      1.00      1.00       240
           1       1.00      1.00      1.00        62
           2       1.00      1.00      1.00       116
           3       1.00      1.00      1.00       113
           4       1.00      1.00      1.00       109

    accuracy                           1.00       640
   macro avg       1.00      1.00      1.00       640
weighted avg       1.00      1.00      1.00       640
```

Scores for each fold using training data (PCA, Logistic Regression, StratifiedKFold)



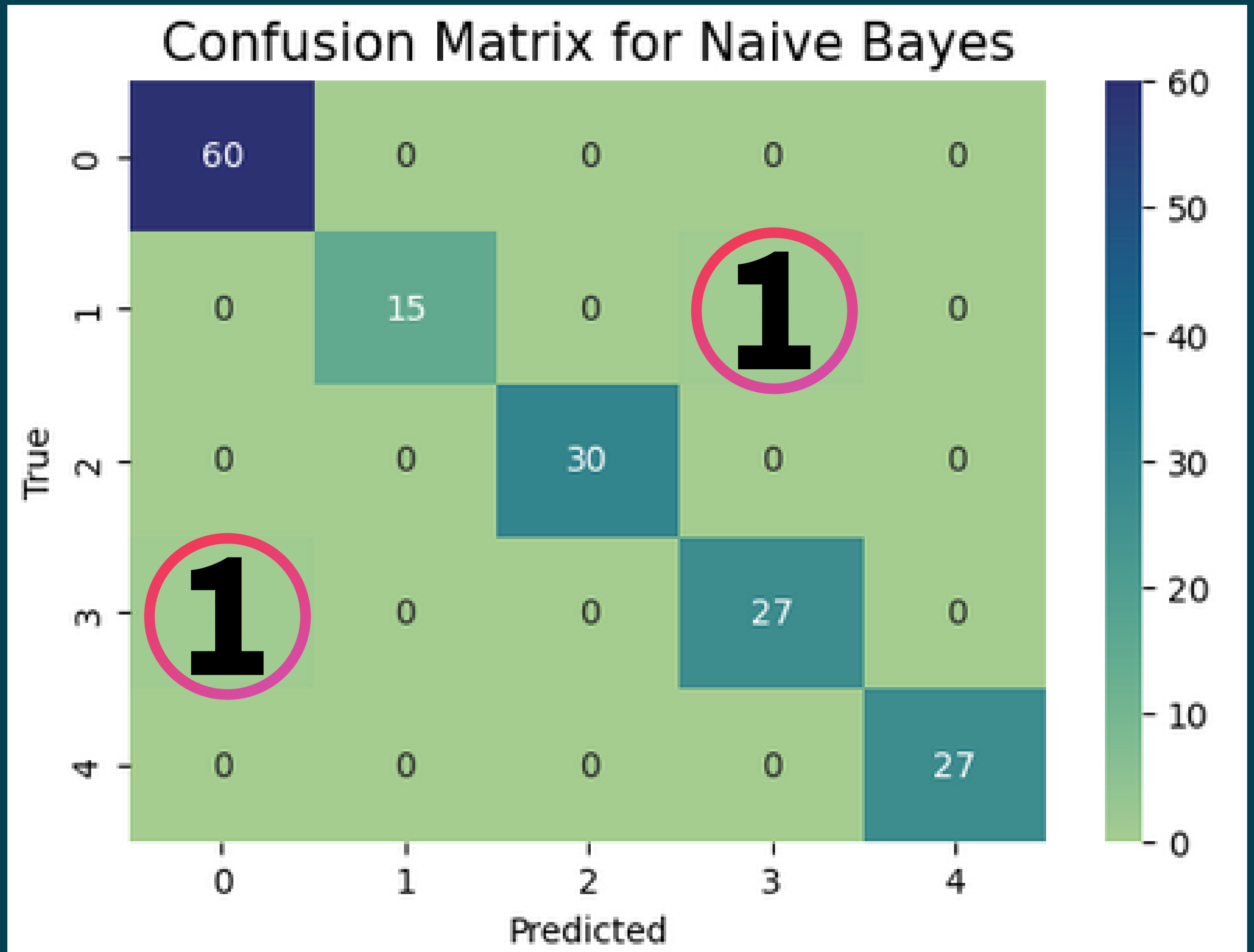
```
Fold number: 0, F1_macro_avg: 0.991
Fold number: 1, F1_macro_avg: 1.000
Fold number: 2, F1_macro_avg: 1.000
Fold number: 3, F1_macro_avg: 0.993
Fold number: 4, F1_macro_avg: 0.991
```



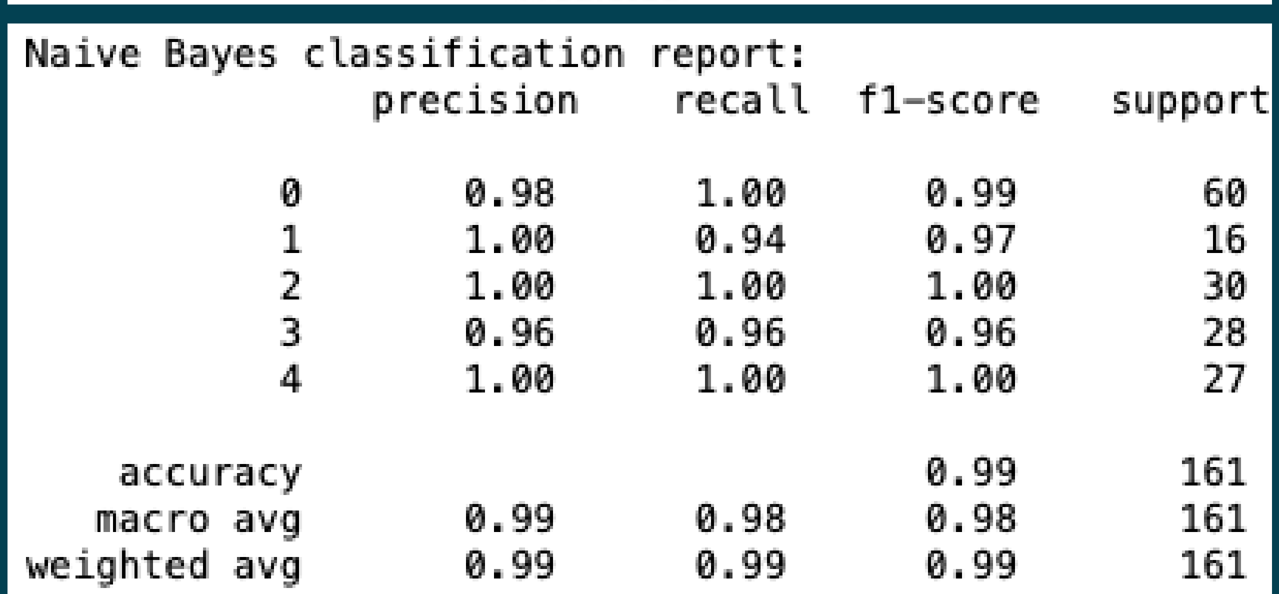
```
Test set classification report:
              precision    recall  f1-score   support

           0       0.98      1.00      0.99        60
           1       1.00      1.00      1.00        16
           2       1.00      1.00      1.00        30
           3       1.00      0.96      0.98        28
           4       1.00      1.00      1.00        27

    accuracy                           0.99       161
   macro avg       1.00      0.99      0.99       161
weighted avg       0.99      0.99      0.99       161
```

Extended Modeling: *Linear*

Naive Bayes

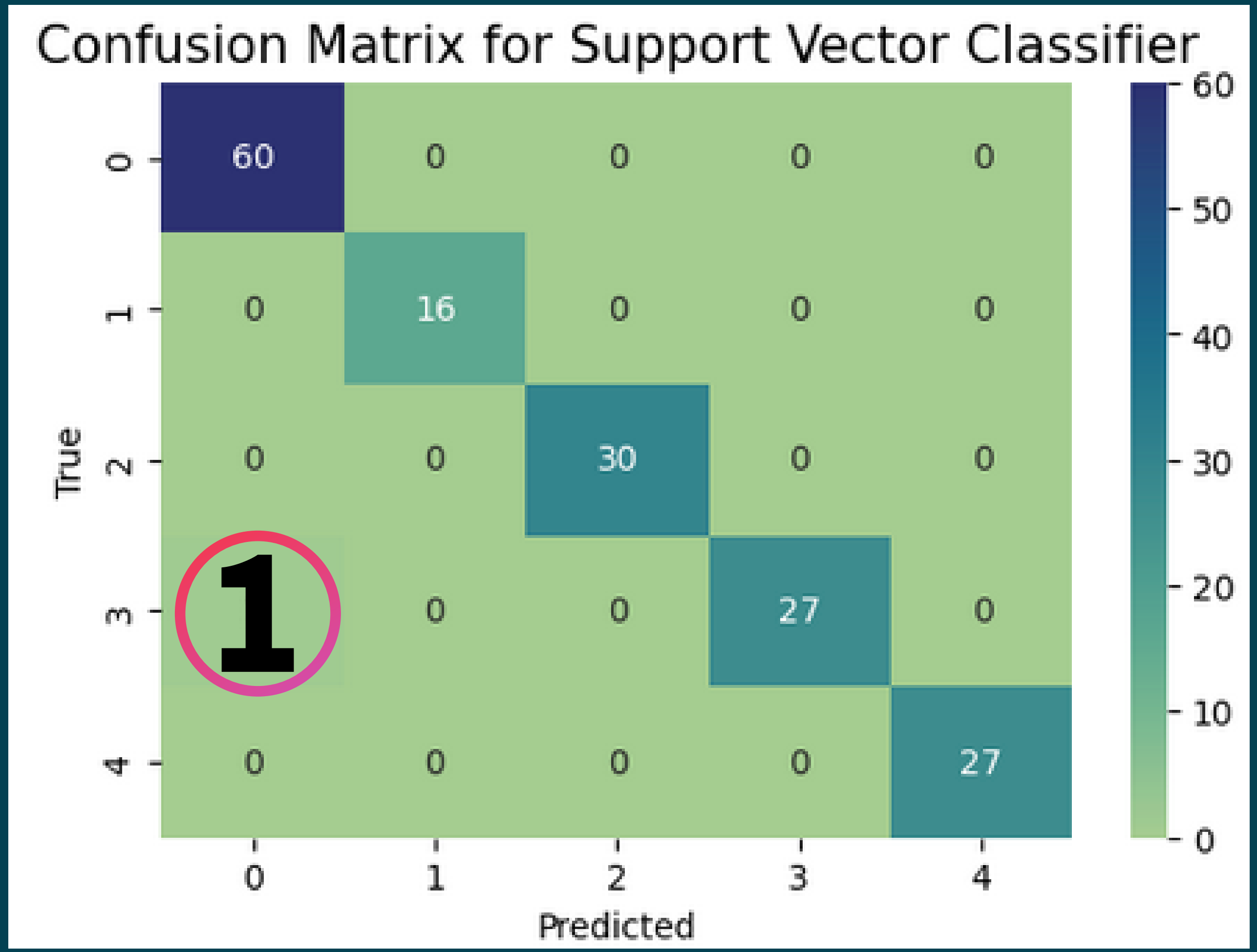


Confusion Matrix for Naive Bayes

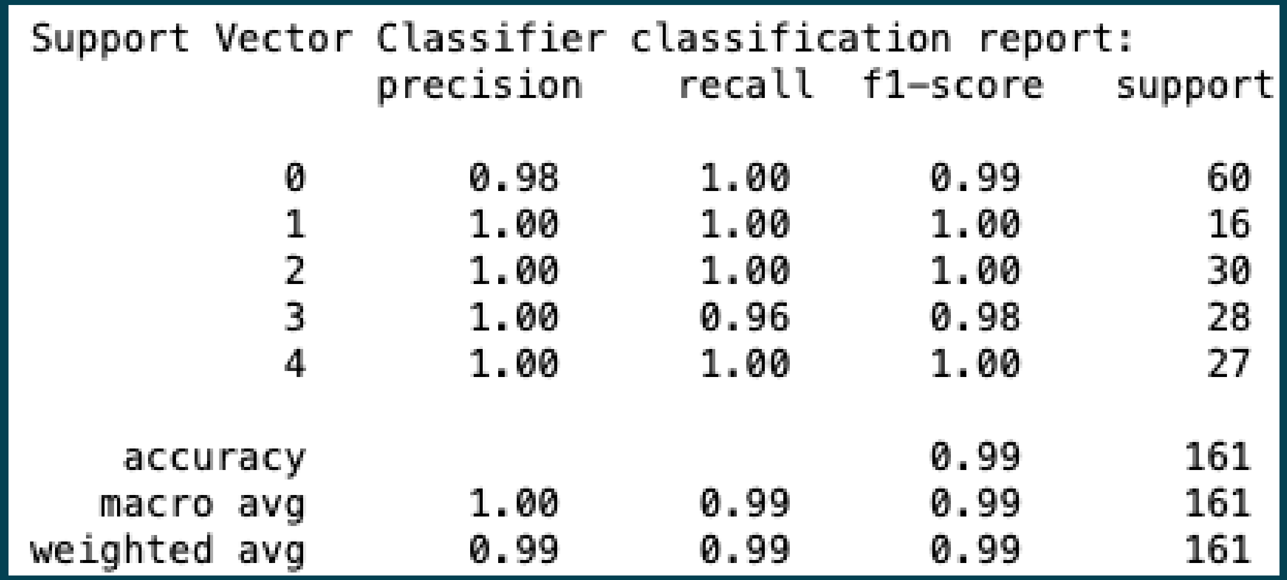


```
Naive Bayes classification report:
              precision    recall  f1-score   support

           0       0.98      1.00      0.99        60
           1       1.00      0.94      0.97        16
           2       1.00      1.00      1.00        30
           3       0.96      0.96      0.96        28
           4       1.00      1.00      1.00        27

    accuracy                           0.99       161
   macro avg       0.99      0.98      0.98       161
weighted avg       0.99      0.99      0.99       161
```

Support Vector Classifier



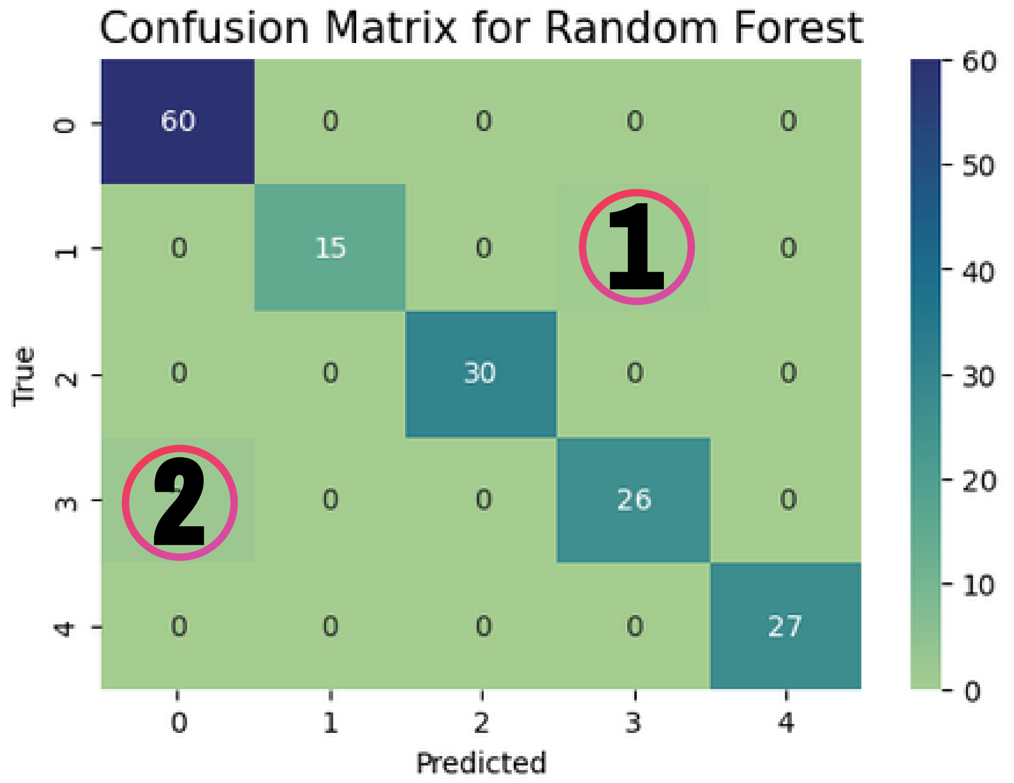
Confusion Matrix for Support Vector Classifier

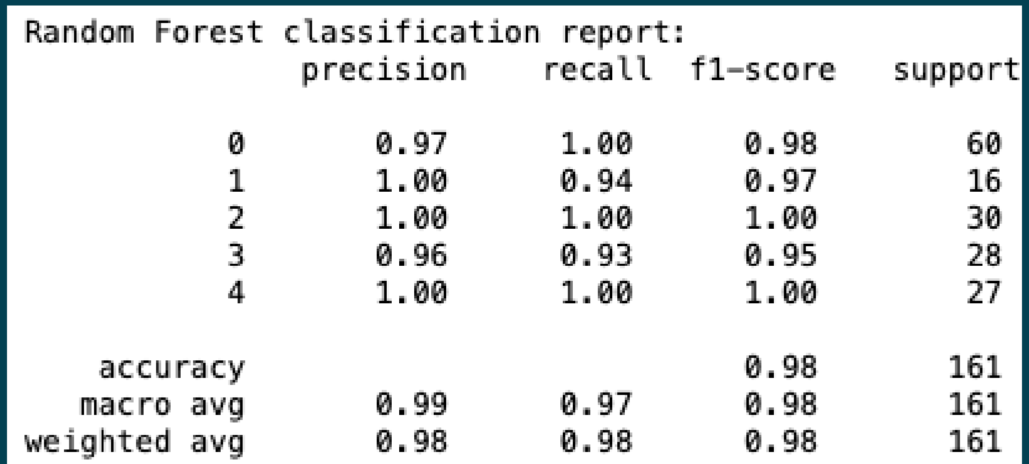


```
Support Vector Classifier classification report:
              precision    recall  f1-score   support

           0       0.98      1.00      0.99        60
           1       1.00      1.00      1.00        16
           2       1.00      1.00      1.00        30
           3       1.00      0.96      0.98        28
           4       1.00      1.00      1.00        27

    accuracy                           0.99       161
   macro avg       1.00      0.99      0.99       161
weighted avg       0.99      0.99      0.99       161
```

Extended Modeling: *Non-linear* *with hyper-parameter tuning*

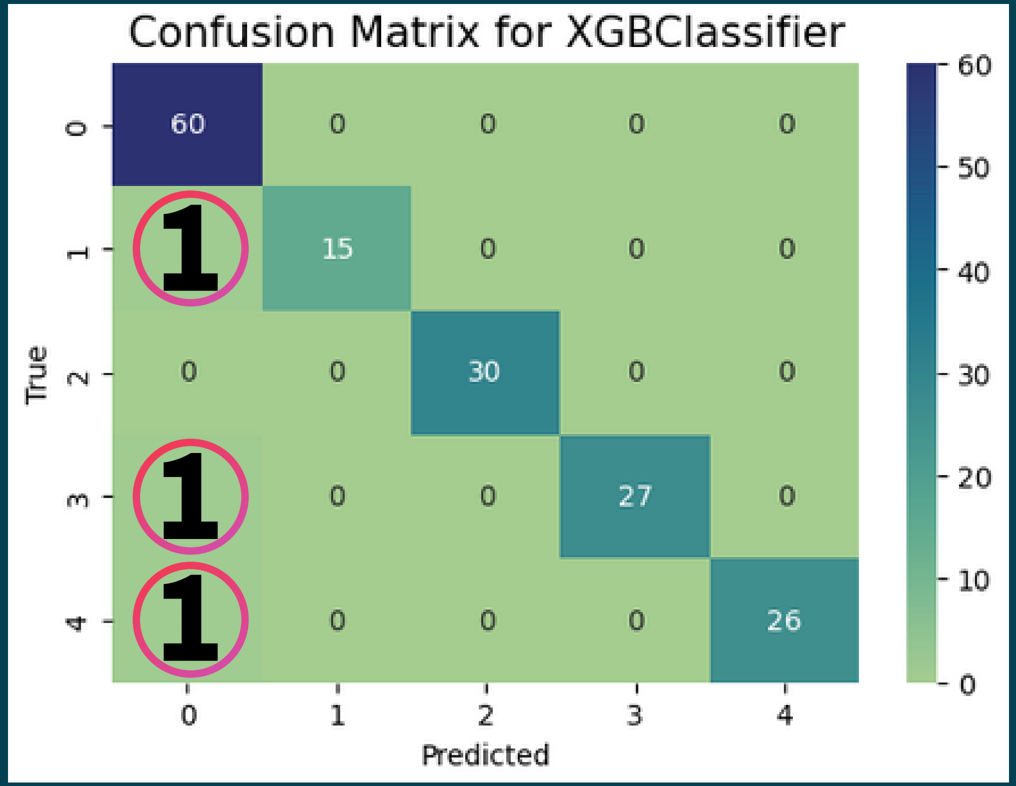
Random Forest Classifier

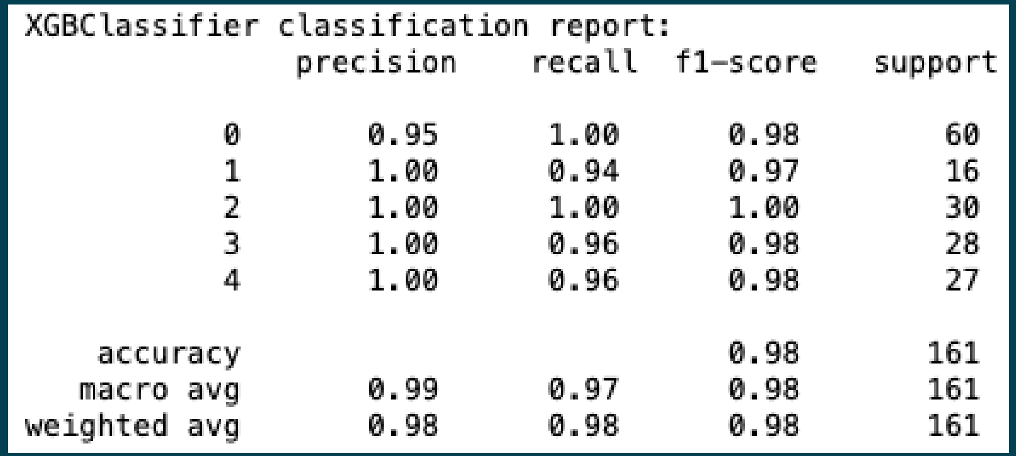




```
Random Forest classification report:
              precision    recall  f1-score   support

           0       0.97      1.00      0.98        60
           1       1.00      0.94      0.97        16
           2       1.00      1.00      1.00        30
           3       0.96      0.93      0.95        28
           4       1.00      1.00      1.00        27

    accuracy                           0.98       161
   macro avg       0.99      0.97      0.98       161
weighted avg       0.98      0.98      0.98       161
```

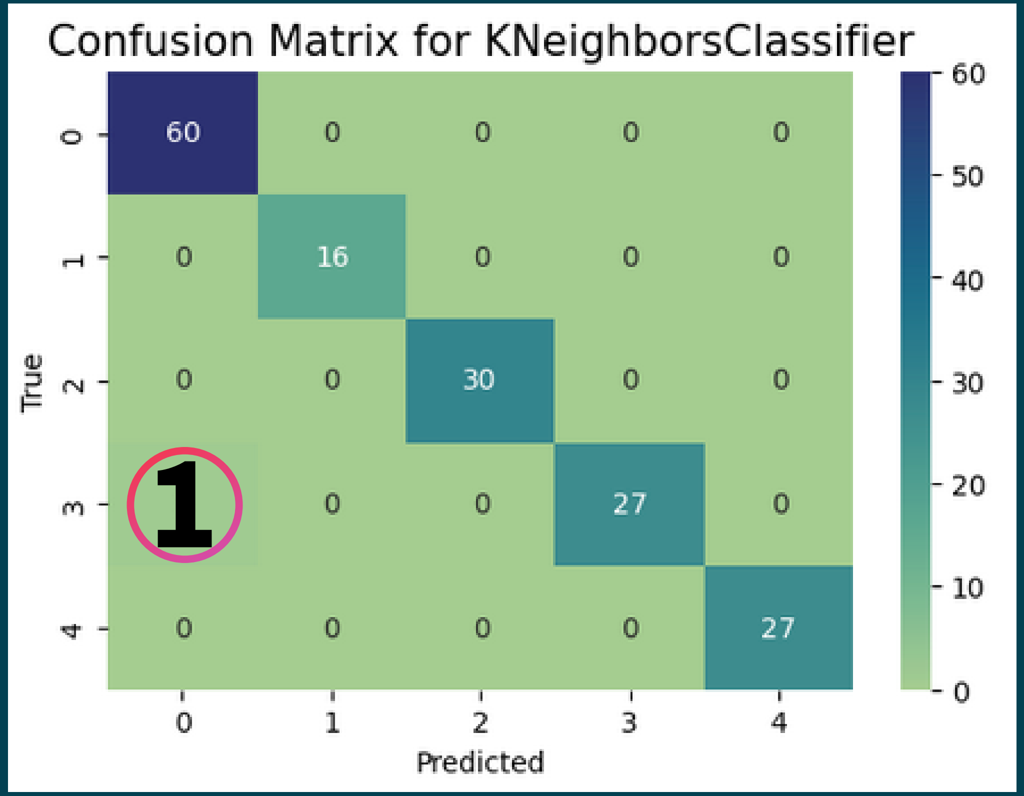
XGBoost Classifier

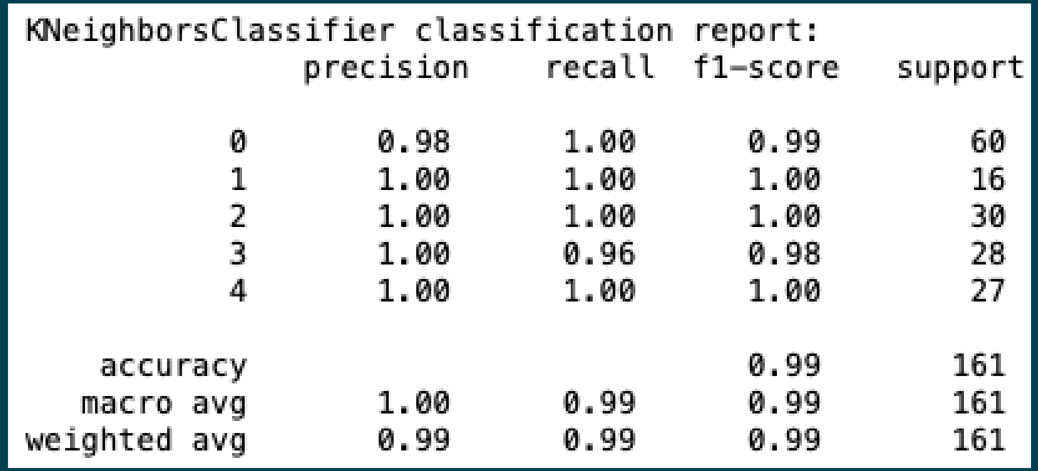




```
XGBClassifier classification report:
              precision    recall  f1-score   support

           0       0.95      1.00      0.98        60
           1       1.00      0.94      0.97        16
           2       1.00      1.00      1.00        30
           3       1.00      0.96      0.98        28
           4       1.00      0.96      0.98        27

    accuracy                           0.98       161
   macro avg       0.99      0.97      0.98       161
weighted avg       0.98      0.98      0.98       161
```

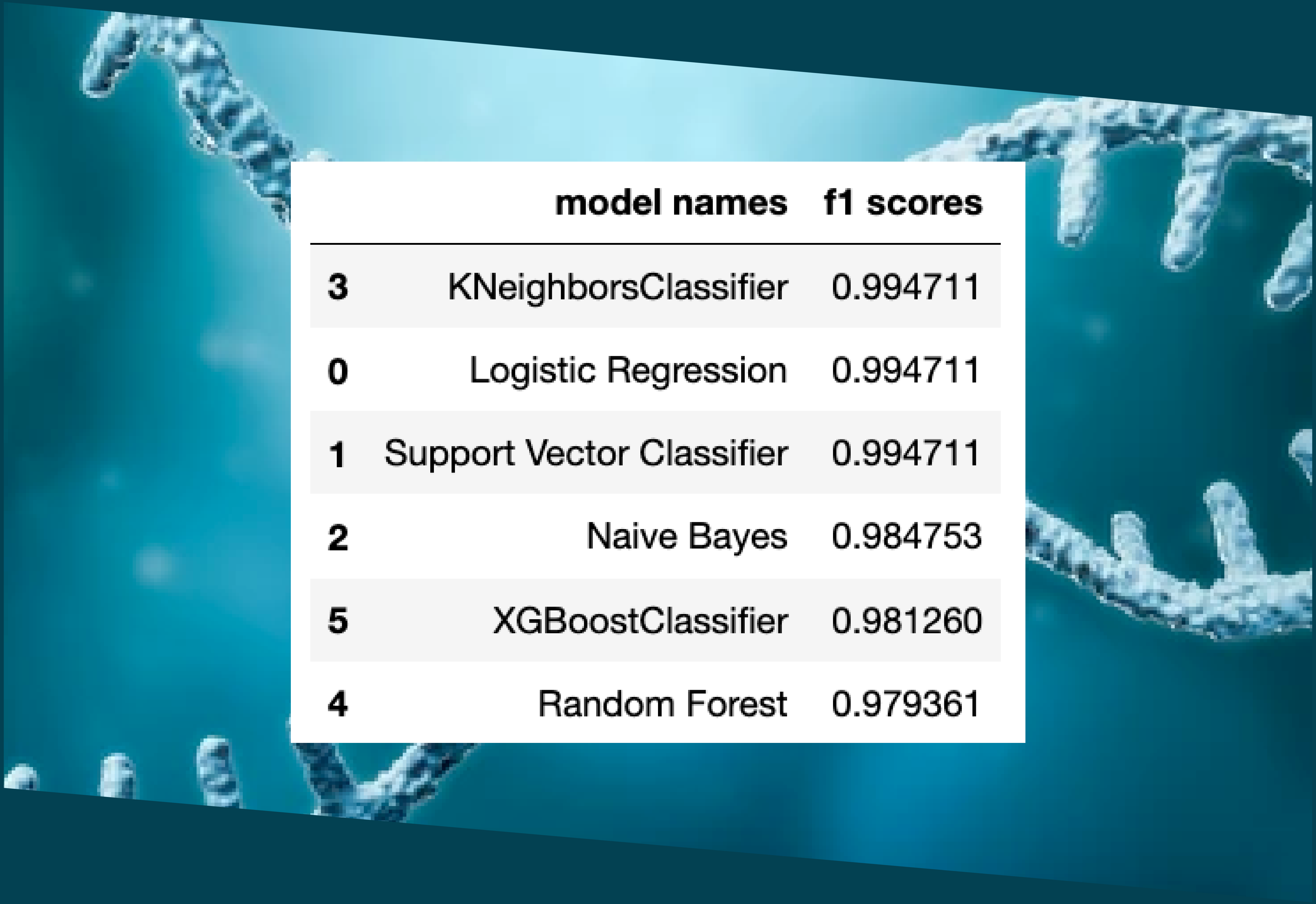
N Neighbors Classifier





```
KNeighborsClassifier classification report:
              precision    recall  f1-score   support

           0       0.98      1.00      0.99        60
           1       1.00      1.00      1.00        16
           2       1.00      1.00      1.00        30
           3       1.00      0.96      0.98        28
           4       1.00      1.00      1.00        27

    accuracy                           0.99       161
   macro avg       1.00      0.99      0.99       161
weighted avg       0.99      0.99      0.99       161
```

Model Comparison: *f1 macro scores*

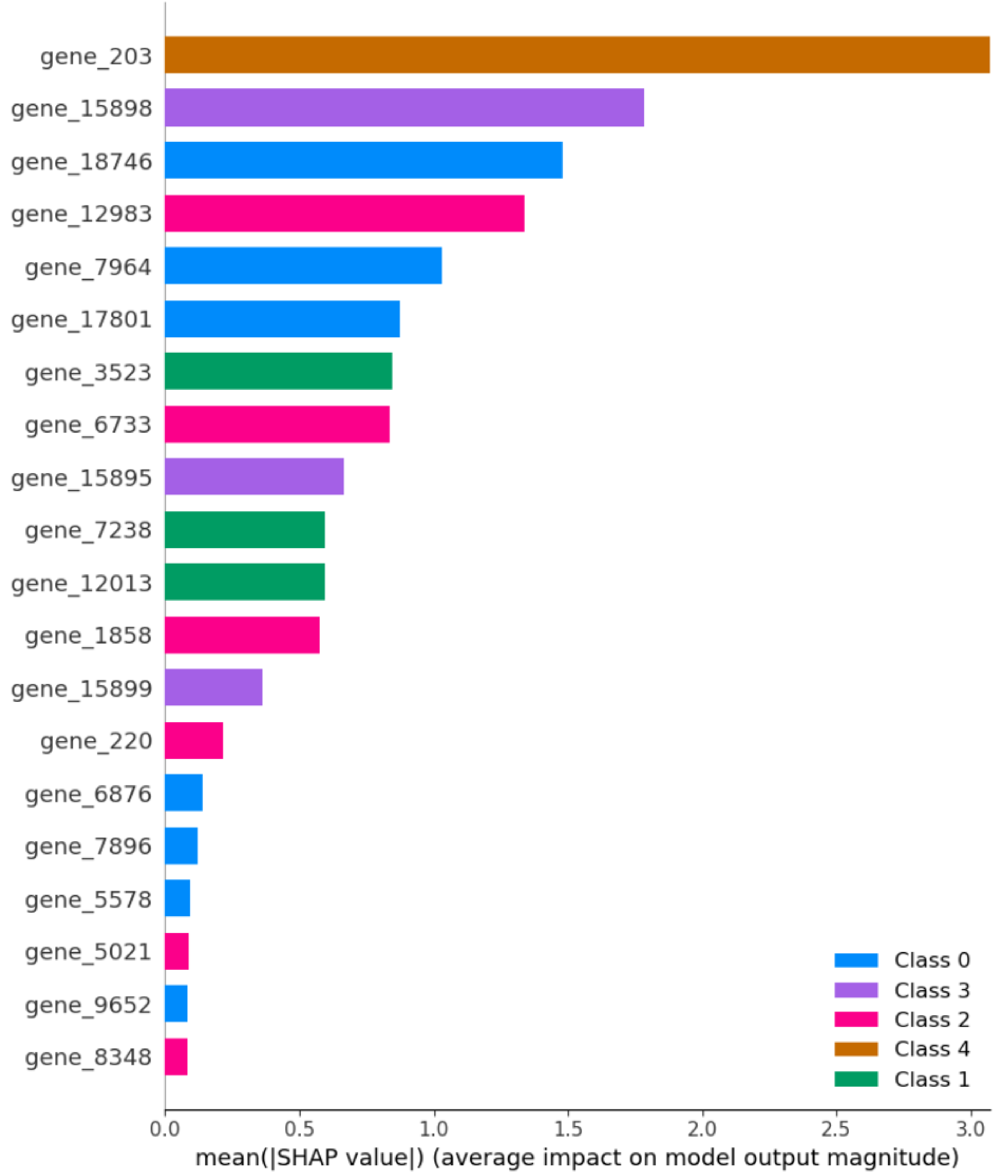


	model names	f1 scores
3	KNeighborsClassifier	0.994711
0	Logistic Regression	0.994711
1	Support Vector Classifier	0.994711
2	Naive Bayes	0.984753
5	XGBoostClassifier	0.981260
4	Random Forest	0.979361

Interpretion:

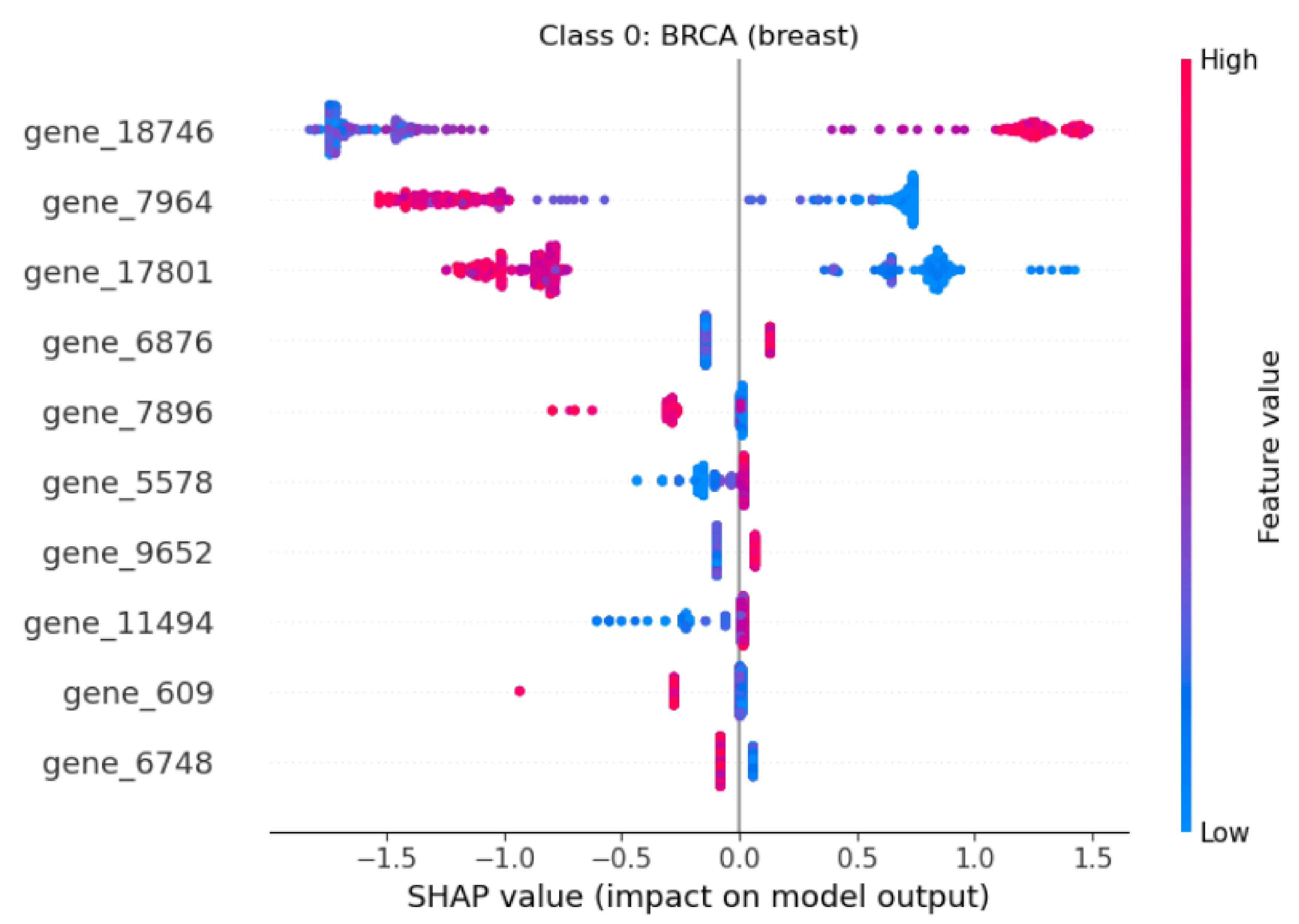
XGBoost Classifier and SHAP

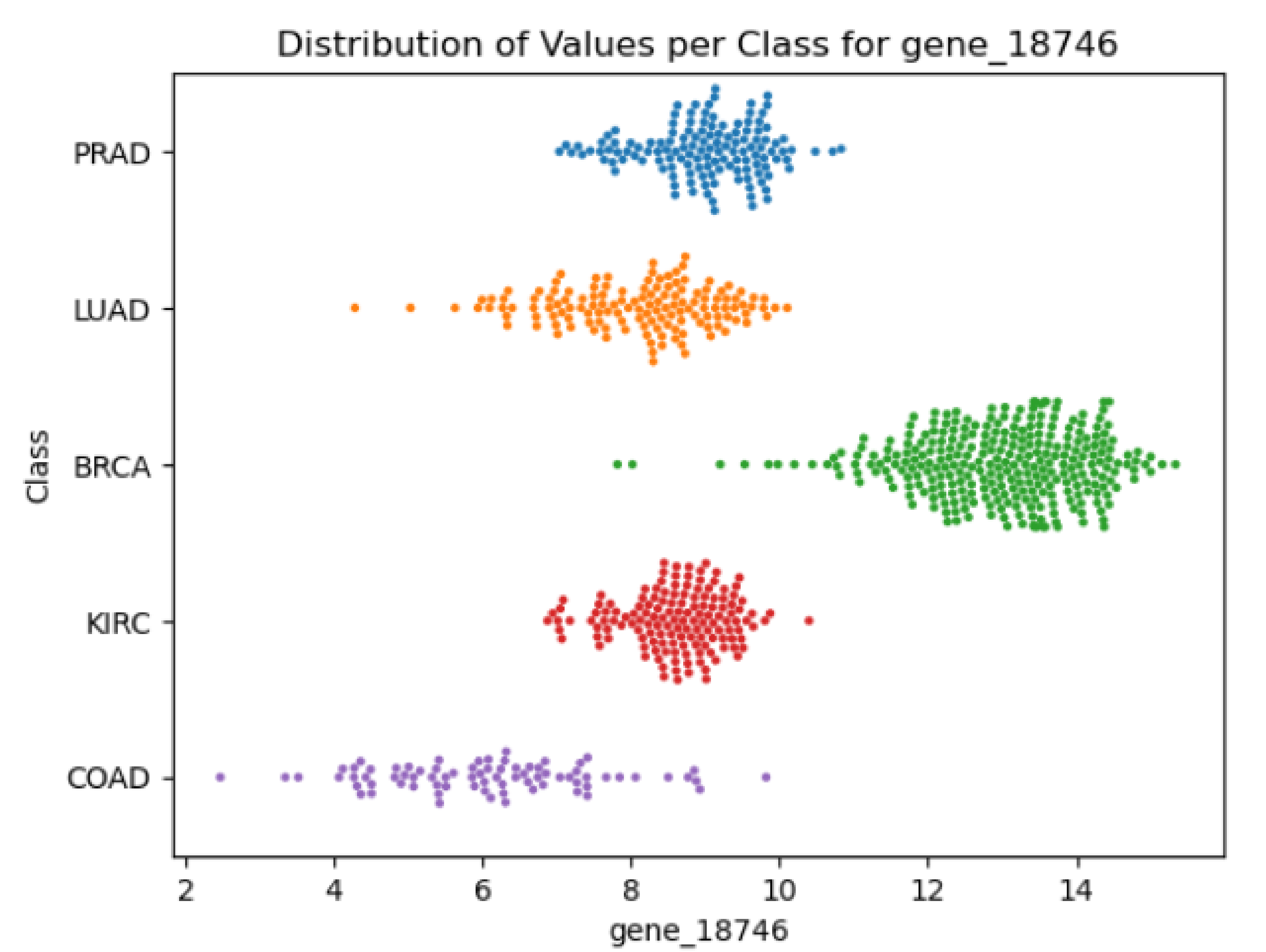
Feature Importance per class

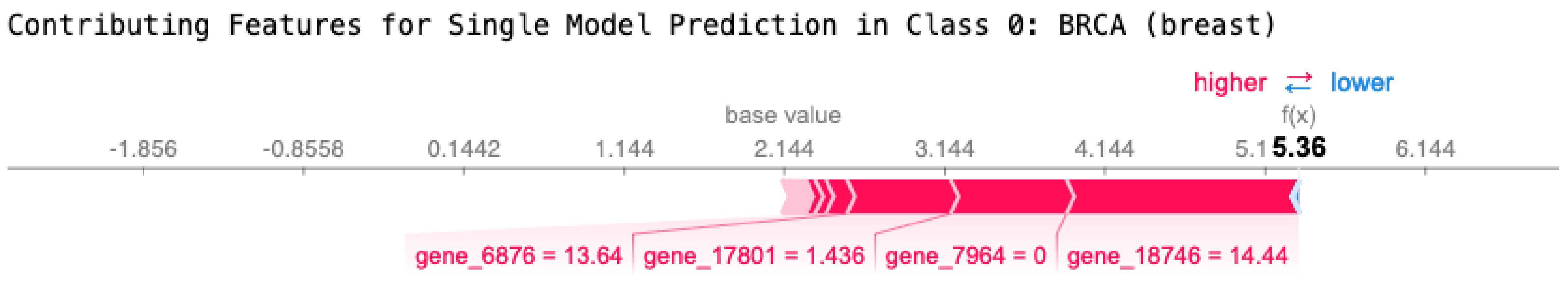


Tamara Horne
2023 | May

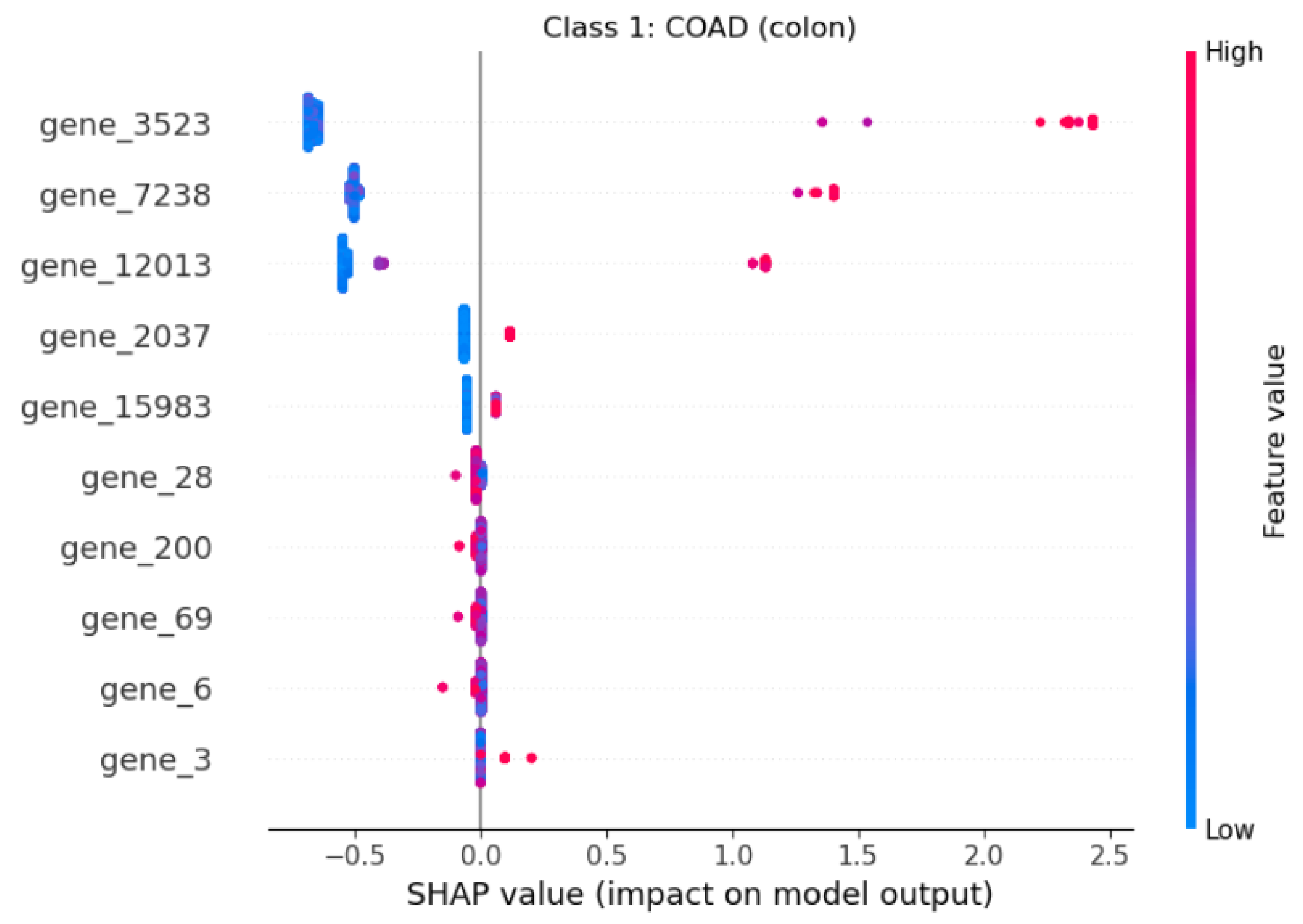
BRCA (breast): *Class 0*

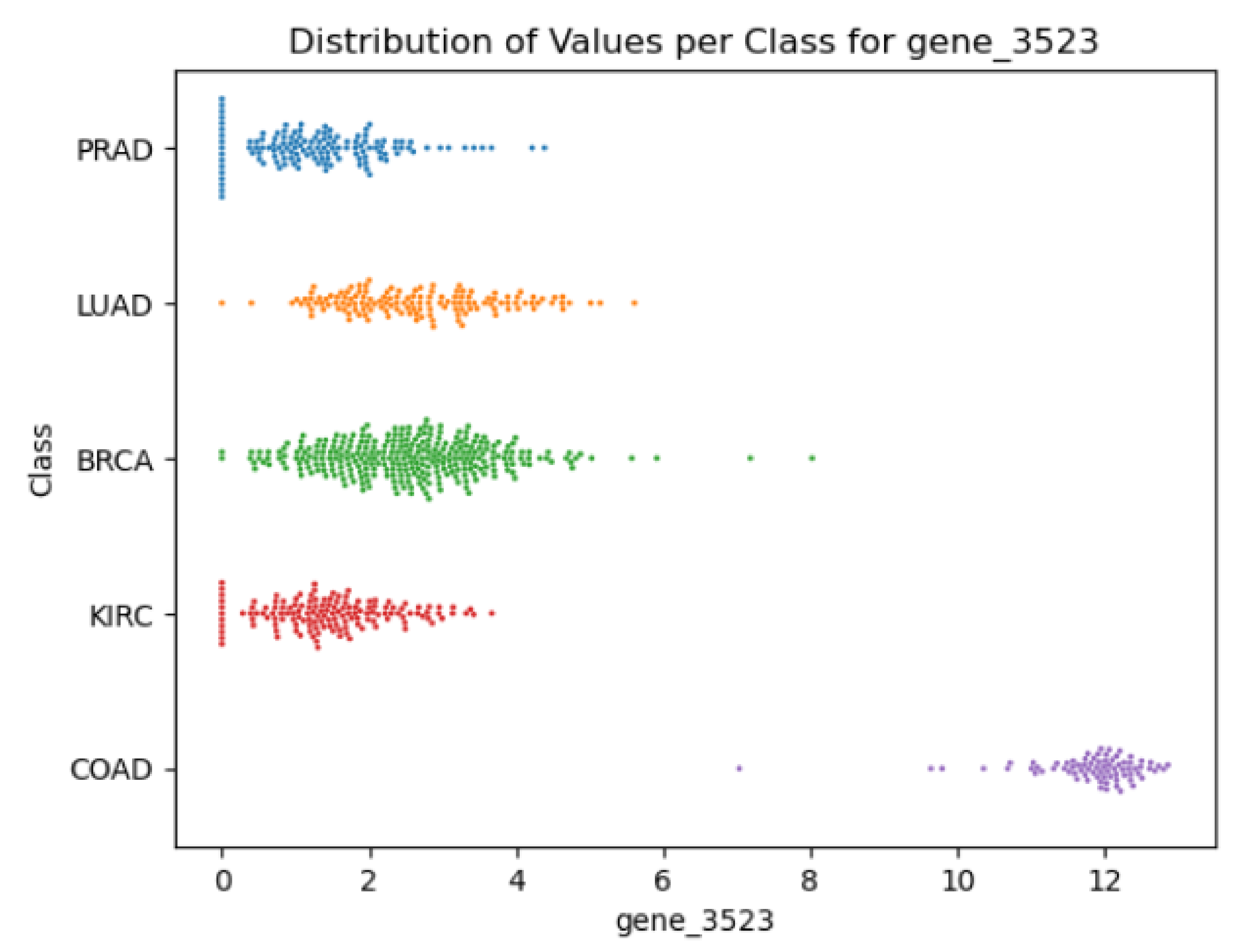


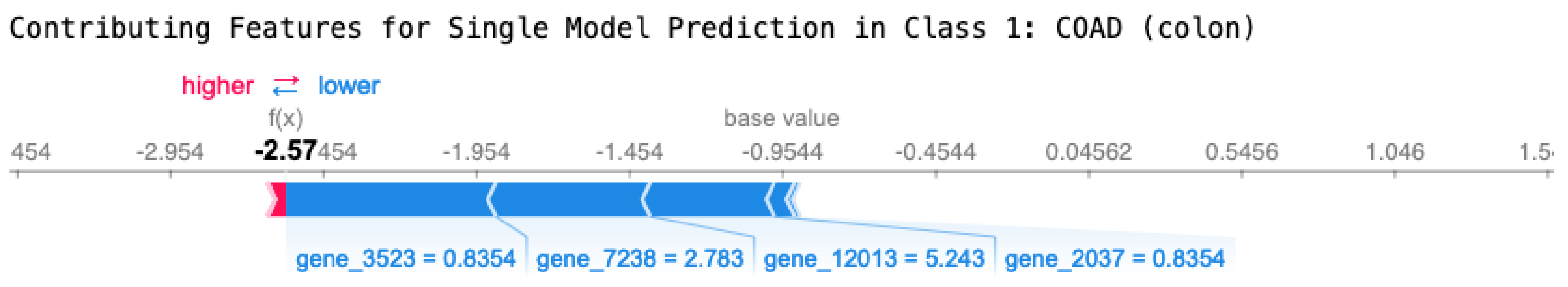




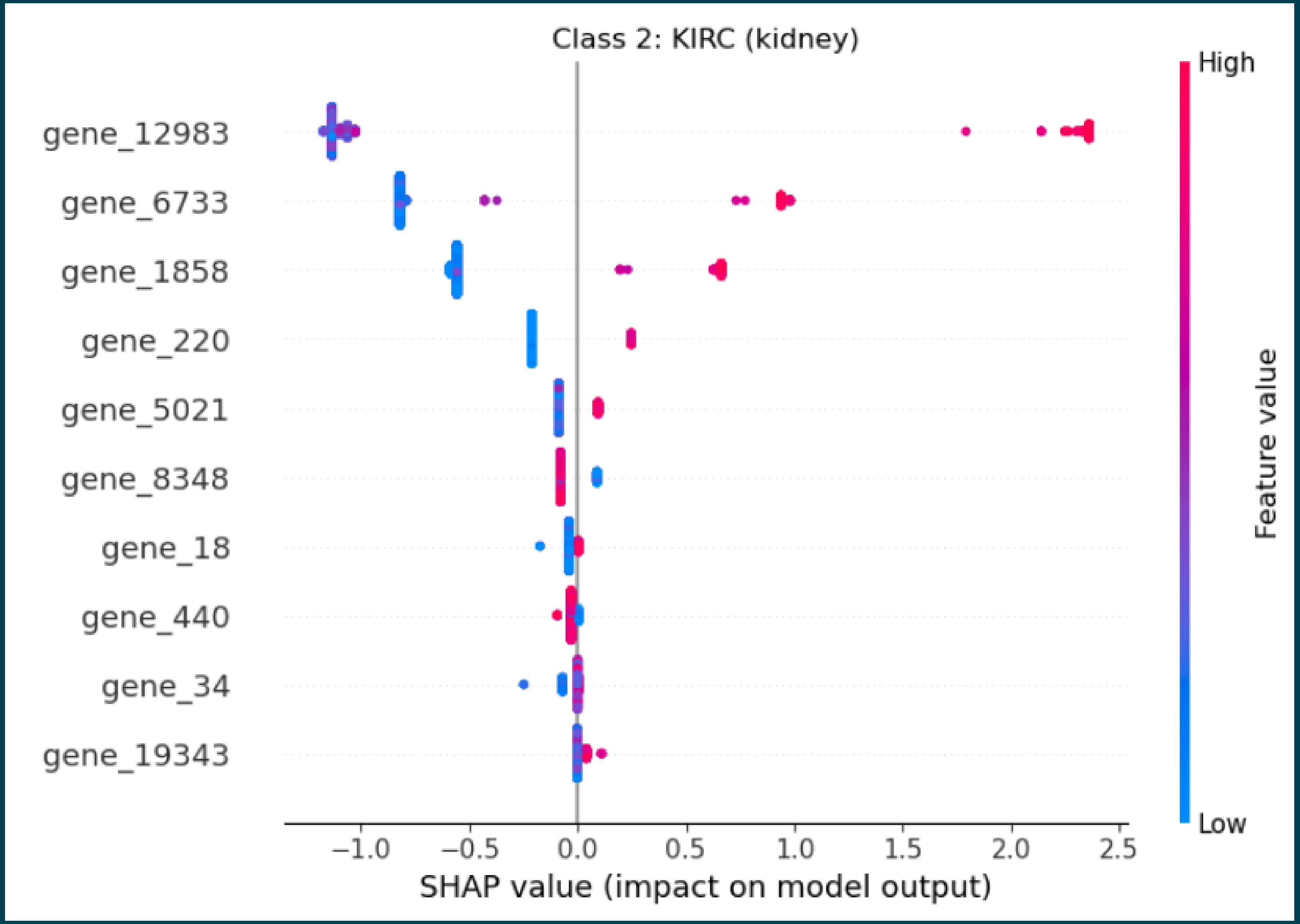
COAD (colon): *Class 1*

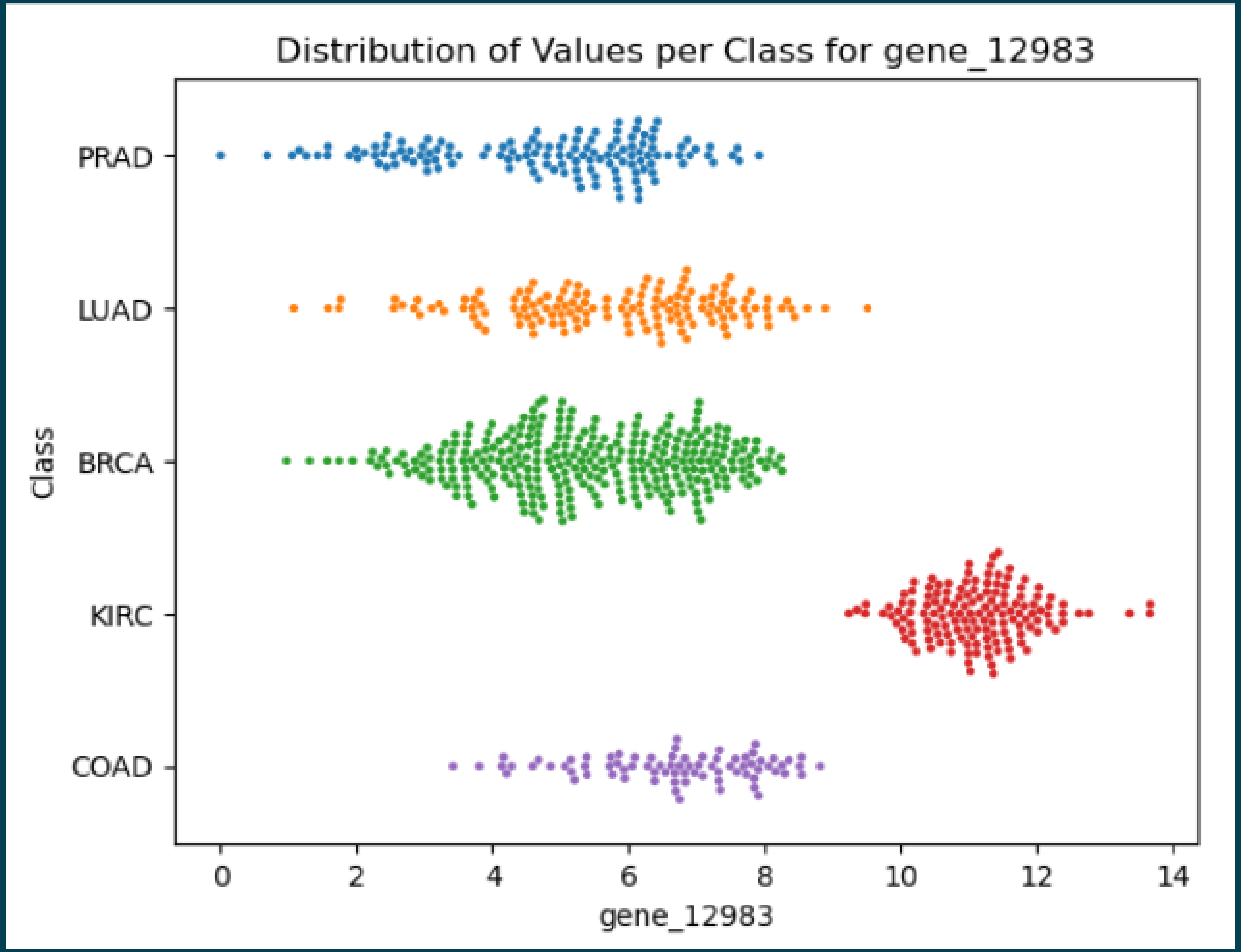


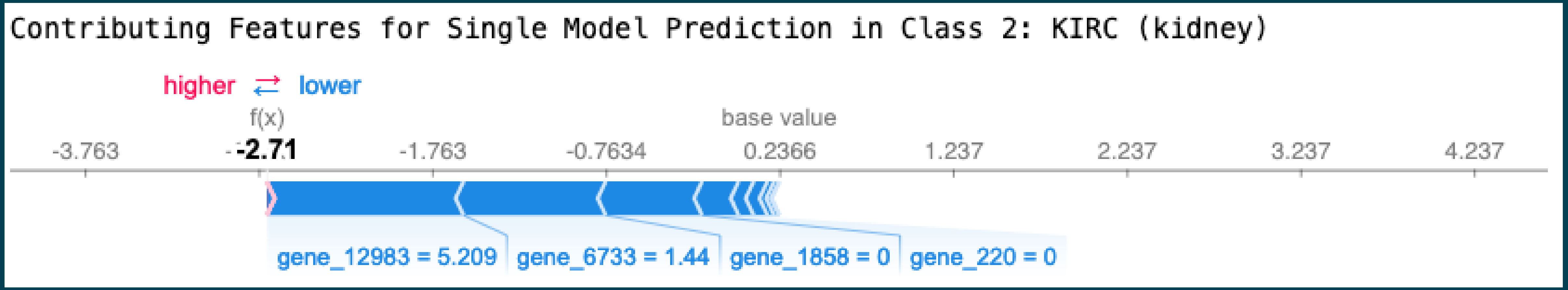




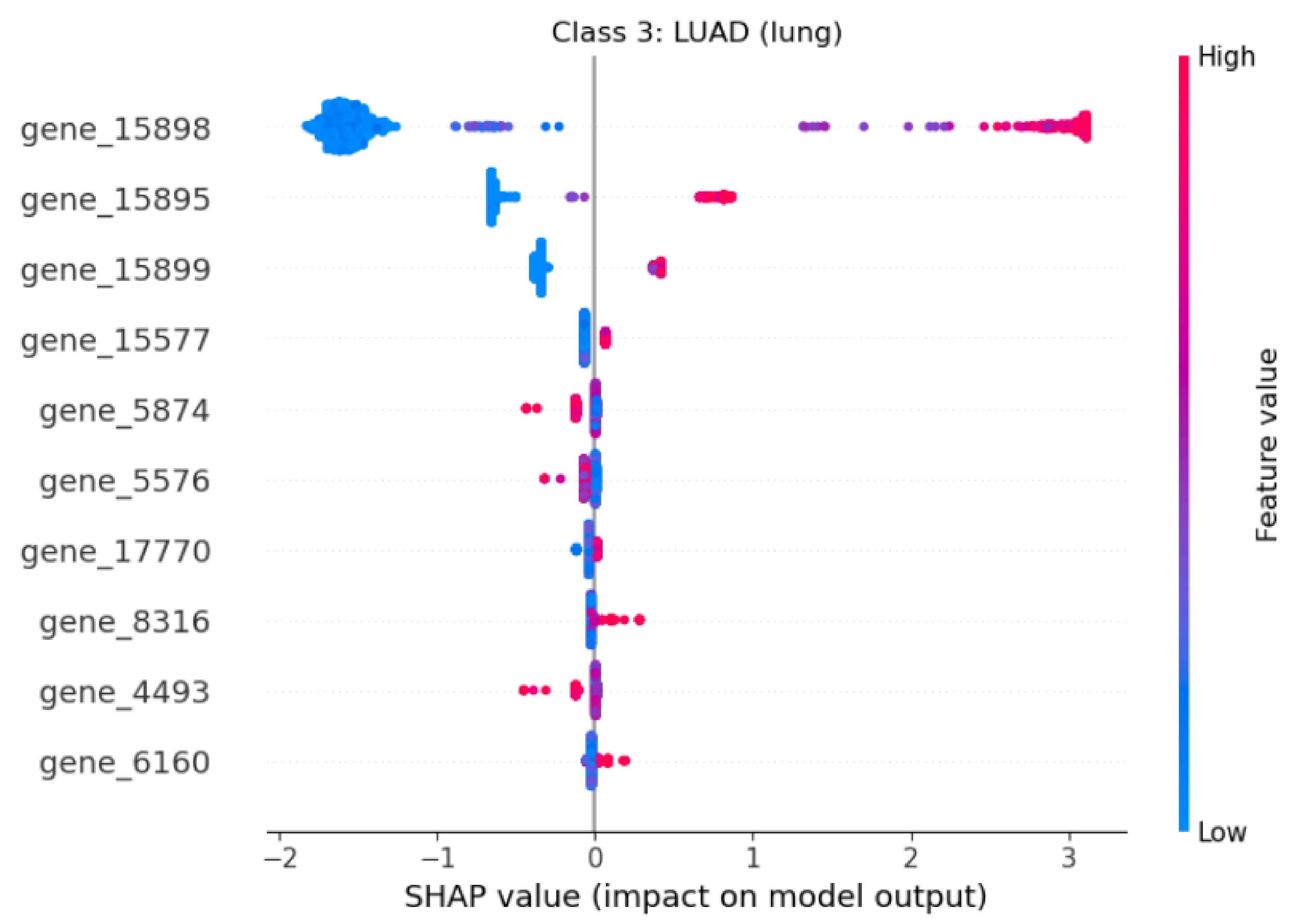
KIRC (kidney): *Class 2*

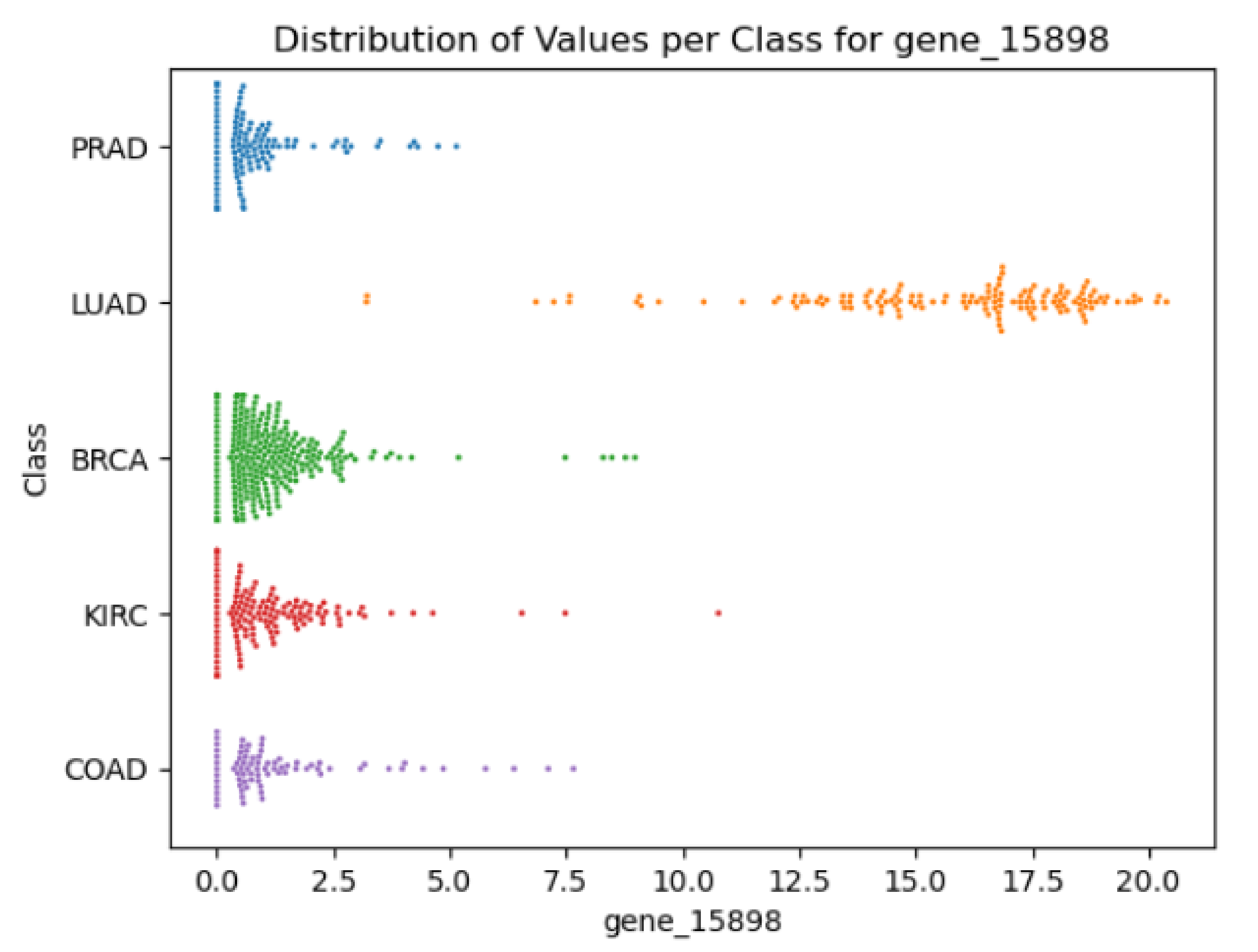




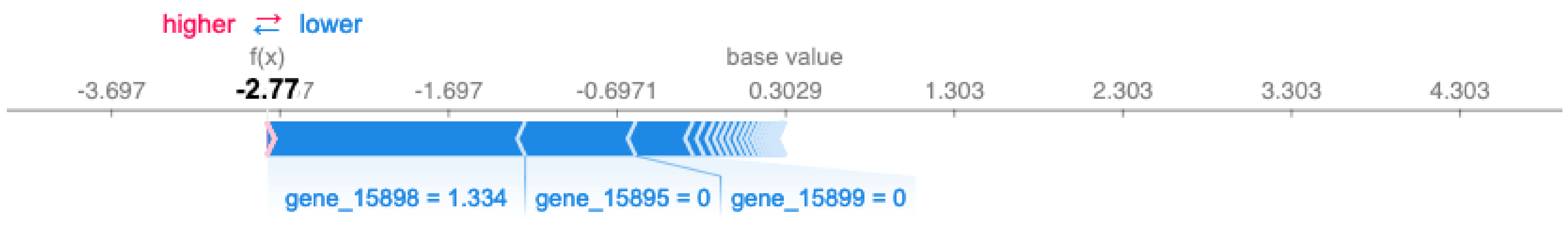


LUAD (lung): *Class 3*



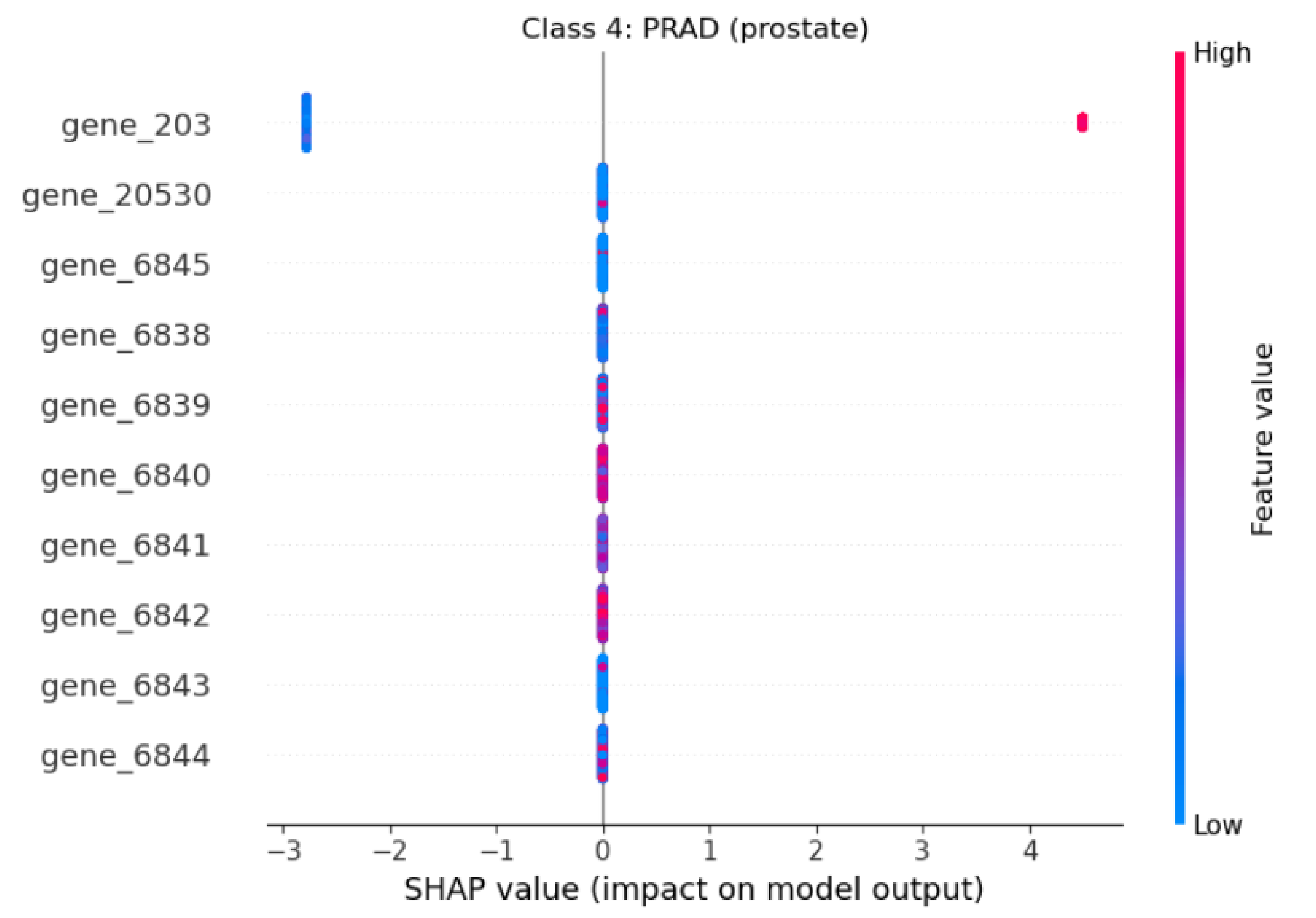


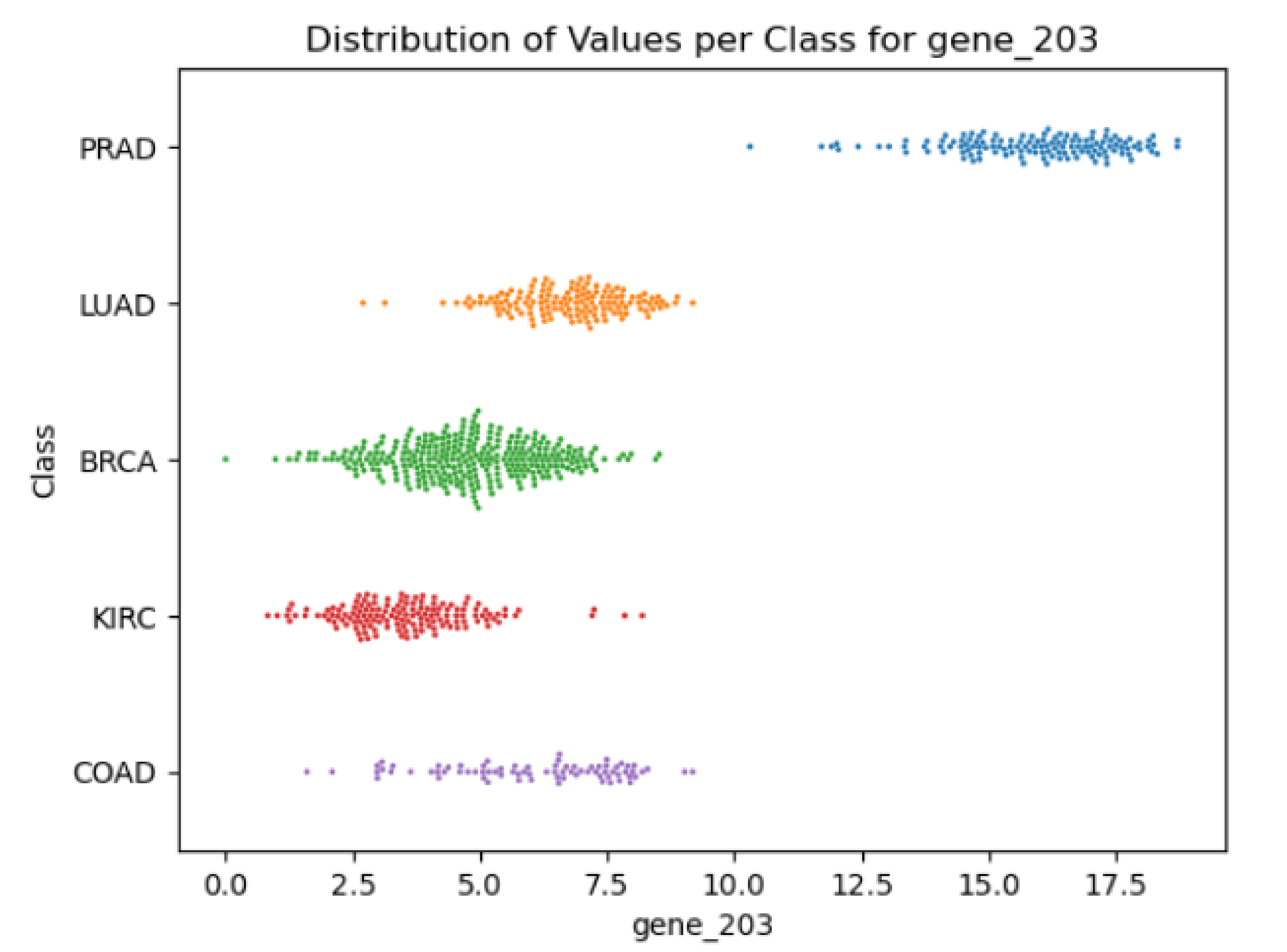
Contributing Features for Single Model Prediction in Class 3: LUAD (lung)

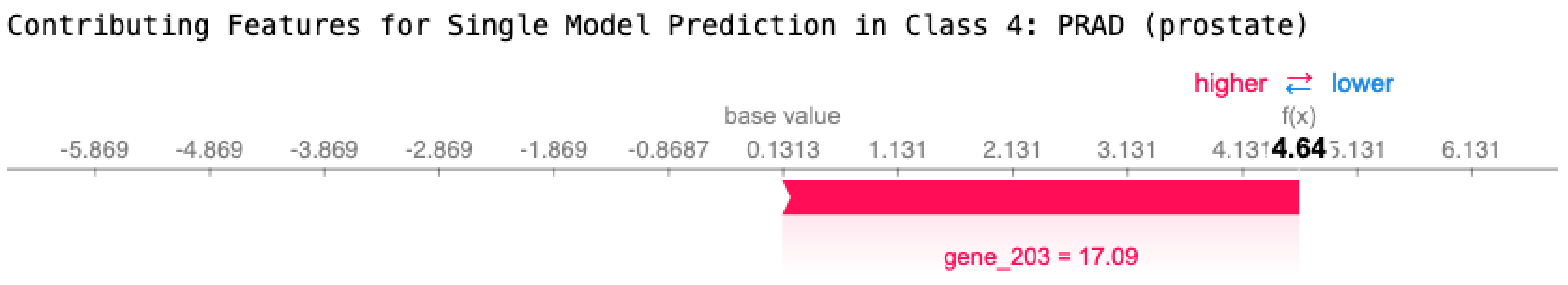


Tamara Horne
2023 | May

PRAD (prostate): *Class 4*



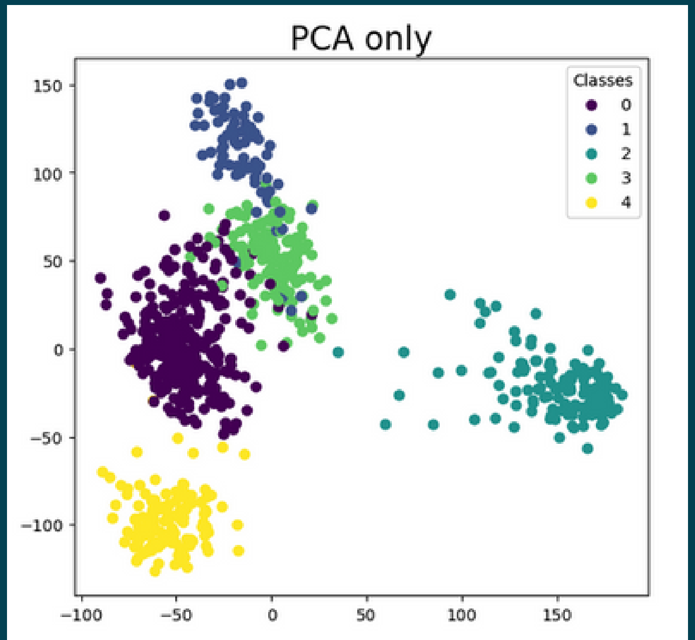


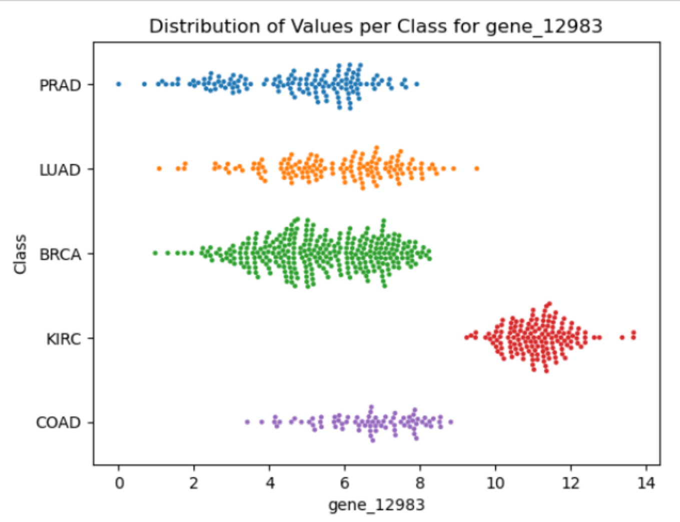


Tamara Horne
2023 | May

Data Predictability *Skepticism of Model Success*

All models had f1 macro scores of over 97%. Why are the classes so easy to predict?





What I Know

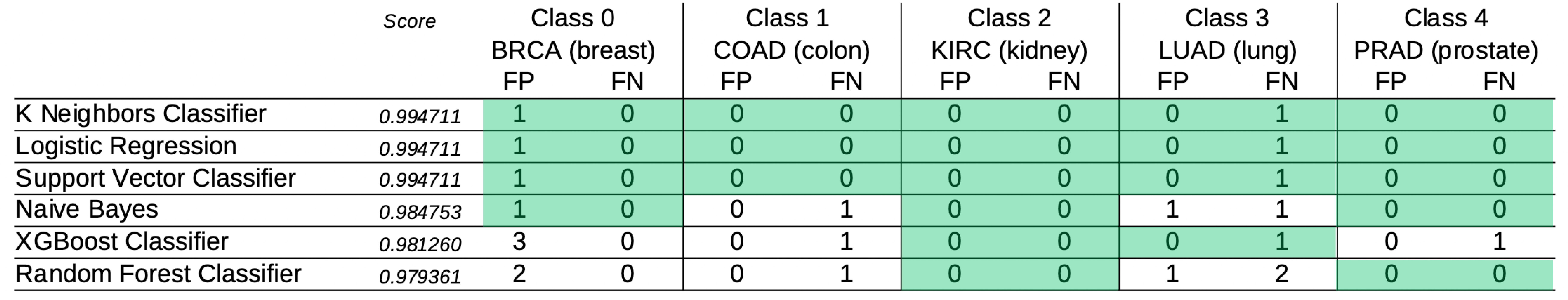
- Classes were largely separate with just two principal components
- Higher values for top feature seen in membership class
- Data comes from a reputable source

What I Don't Know

- In the real world, is there a direct relationship between high gene expression values and cancer class membership? We see a correlation in the data but that cannot be misconstrued for causation.
- Are all gene expression datasets this predictable or is there something abnormal, wrong, or exceptional about this particular dataset?

Conclusions and Client Recommendations

Best Models per Class based on Rate of False Positives/Negatives



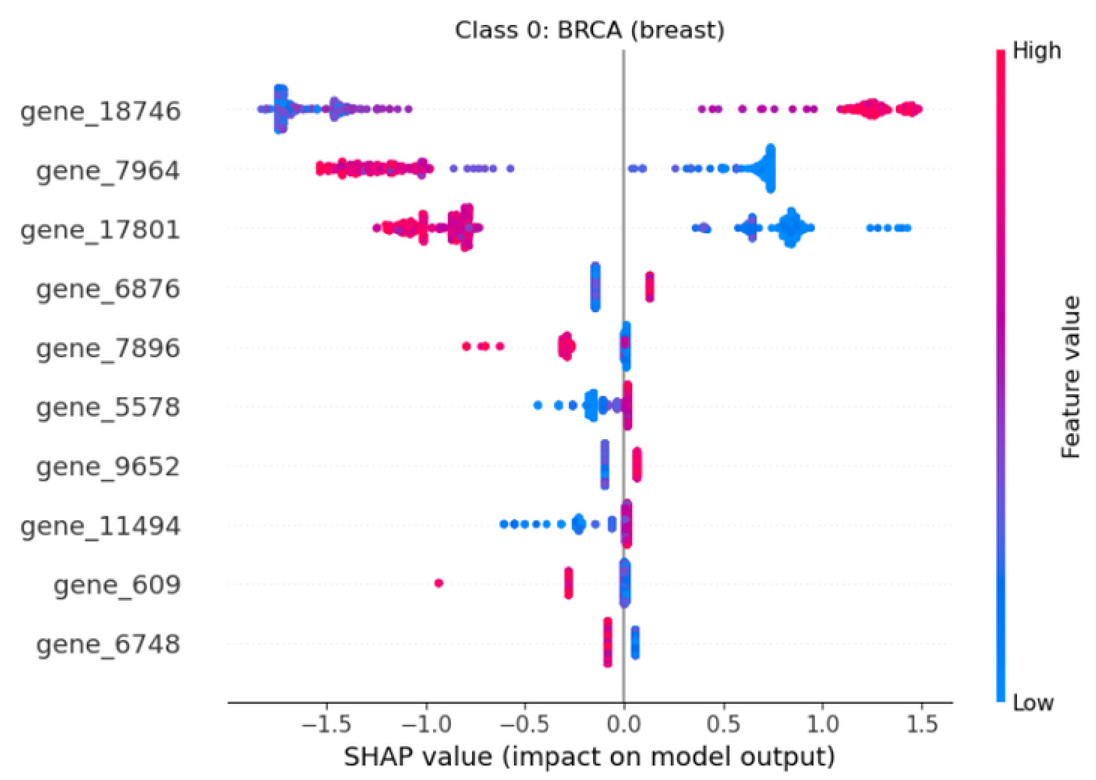
	Score	Class 0		Class 1		Class 2		Class 3		Class 4	
		BRCA (breast)		COAD (colon)		KIRC (kidney)		LUAD (lung)		PRAD (prostate)	
		FP	FN	FP	FN	FP	FN	FP	FN	FP	FN
K Neighbors Classifier	*0.994711*	1	0	0	0	0	0	0	1	0	0
Logistic Regression	*0.994711*	1	0	0	0	0	0	0	1	0	0
Support Vector Classifier	*0.994711*	1	0	0	0	0	0	0	1	0	0
Naive Bayes	*0.984753*	1	0	0	1	0	0	1	1	0	0
XGBoost Classifier	*0.981260*	3	0	0	1	0	0	0	1	0	1
Random Forest Classifier	*0.979361*	2	0	0	1	0	0	1	2	0	0

FP = False Positive (a false positive for class x is one where a true class x sample is predicted to be class y)

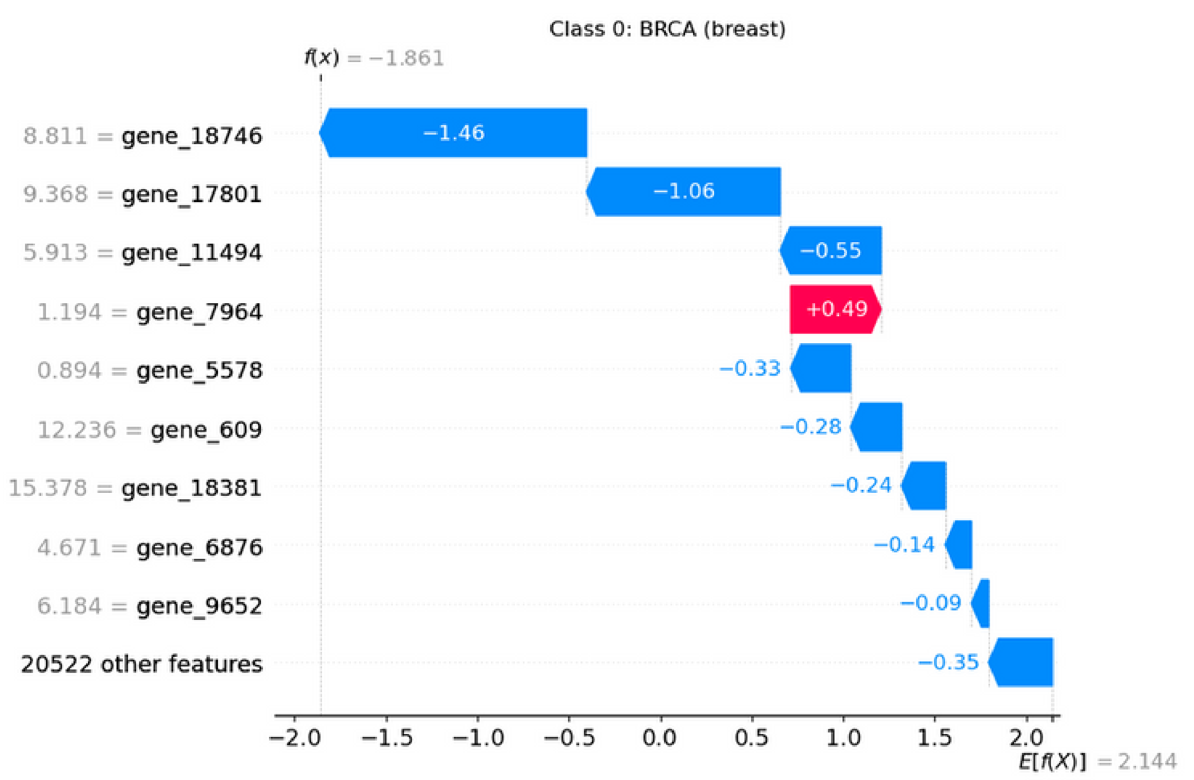
FN = False Negative (a false negative for class x is one where a true class y sample is predicted to be class x)

Conclusions and Client Recommendations

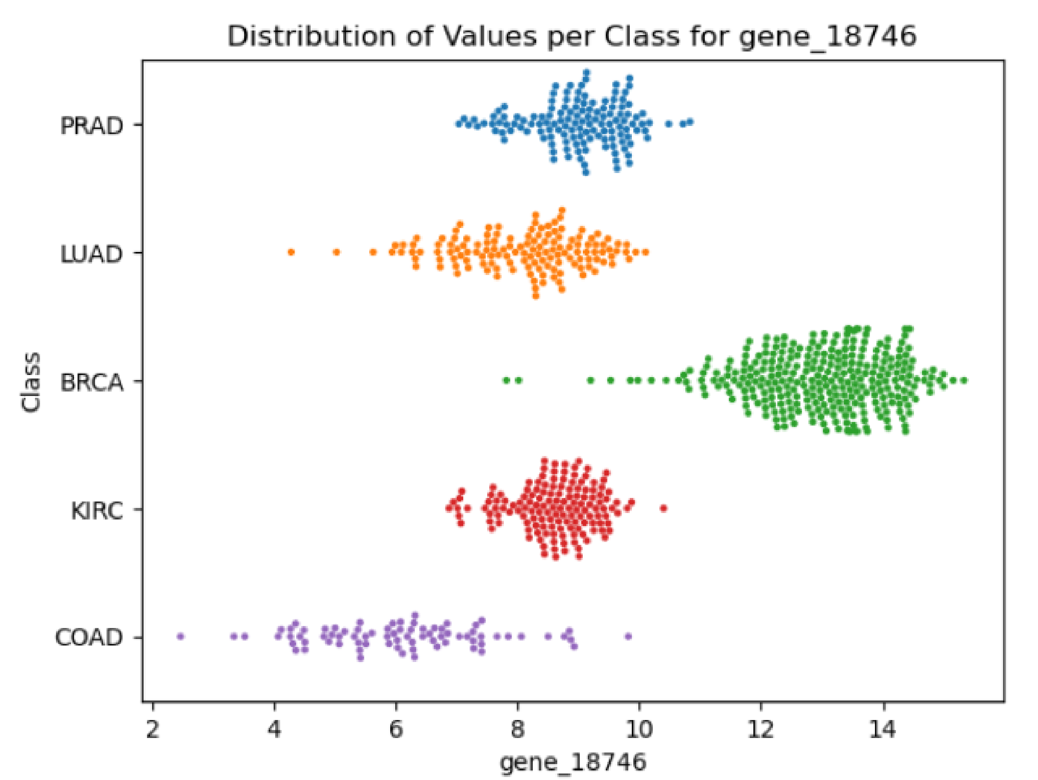
The Knowledge Gained Through Interpretation



Relationship between SHAP values and Feature Importance



Direction and magnitude of feature importance for single sample



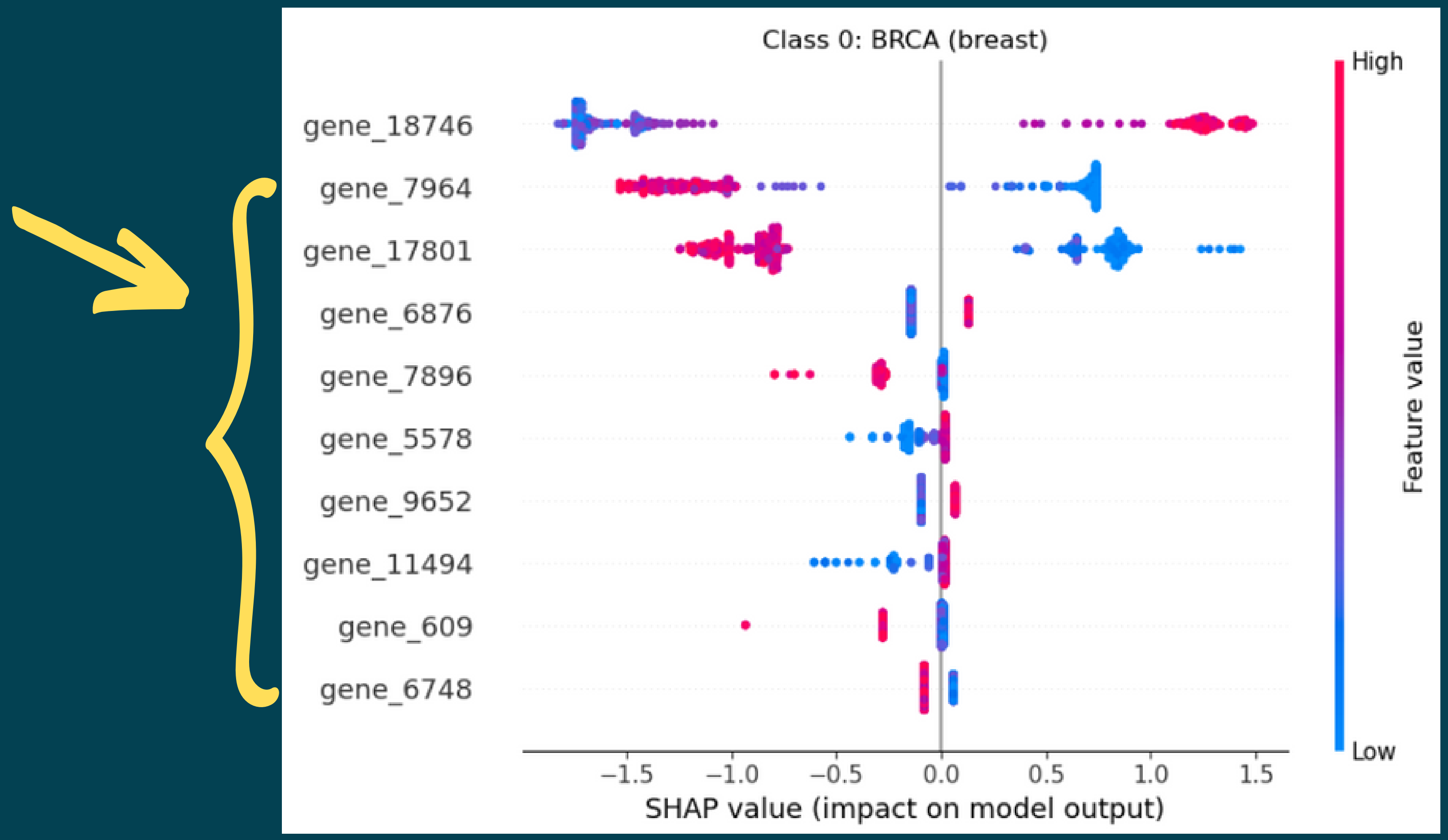
Distribution of values per class for single feature

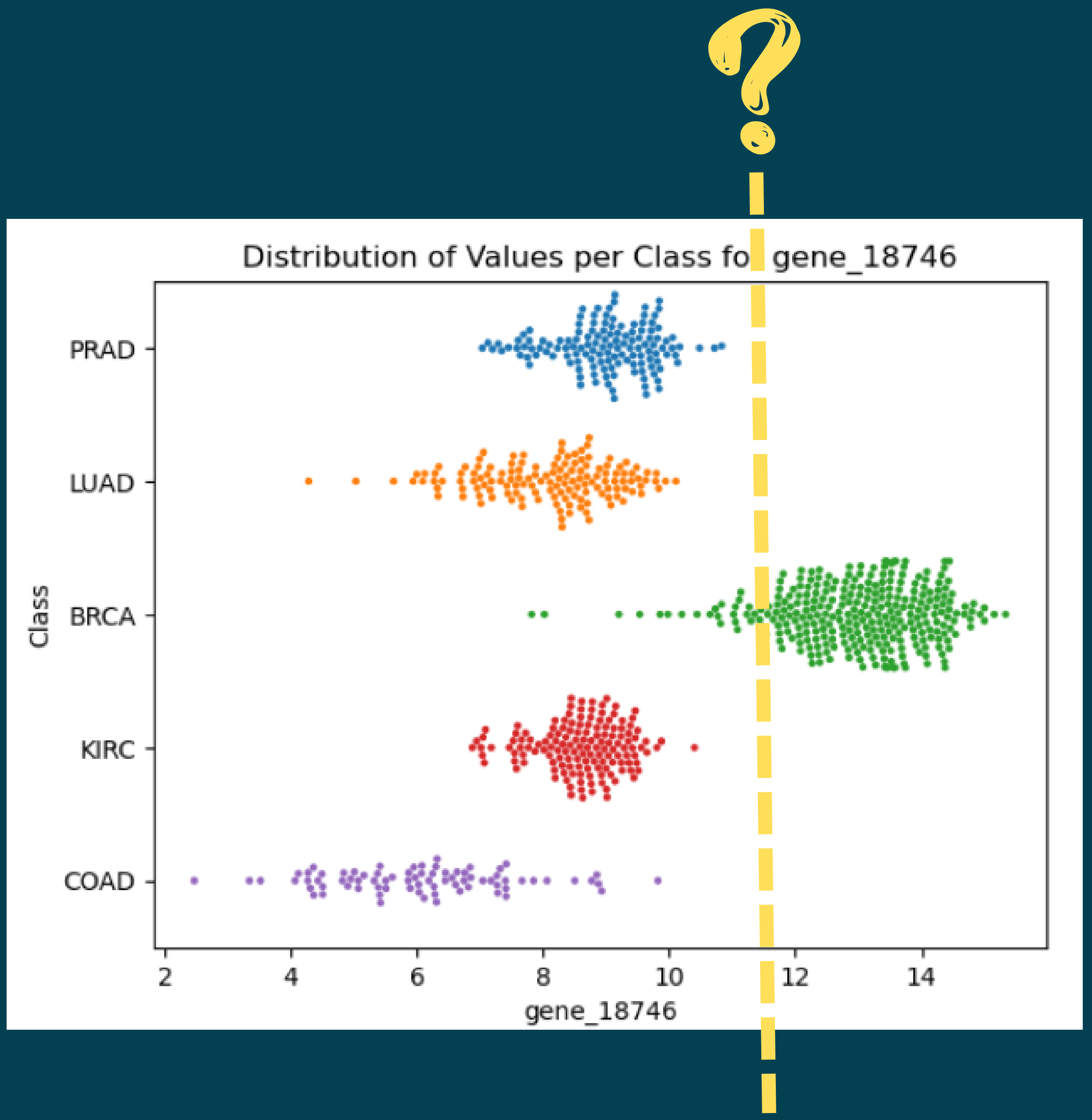
Possible Future Project Extension

Explore each feature in greater depth

- Plot feature gene expression value distribution for the other important features for each class.

- Find value threshold for important features above which there is a 100% chance of class membership.





shutterstock.com 1907619613 royalty free

For More Information Please Visit

https://github.com/tamarahorne/Springboard/tree/main/Capstone%20Project%203