# Feature Selection (FS) workflow report

*Enrique Audain*

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## Introduction

The report summarizing the Feature Selection pipeline results.

## Feature Selection workflow

Univariate canonical correlation (X2) with Recursive Feature Elimination (RFE) wrapped with Random Forest (RF).

## Dataset

Triple-Negative Breast Cancer (TNBC) proteome. Label-free deep proteome analysis of 44 (samples and technical repliques) human breast specimens.

## Summary stats from training phase

Table 1: Best model metrics from 10-folds cross-validation resampling.

| Variables | Accuracy | Kappa | AccuracySD | KappaSD |
|---|---|---|---|---|
| 1 | 0.575 | 0.4511 | 0.3104 | 0.3857 |
| 2 | 0.5167 | 0.3934 | 0.2908 | 0.3356 |
| 3 | 0.7667 | 0.6907 | 0.235 | 0.3094 |
| 4 | 0.6917 | 0.5311 | 0.2637 | 0.42 |
| 5 | 0.7417 | 0.667 | 0.2952 | 0.3793 |
| 6 | 0.6917 | 0.567 | 0.2888 | 0.4122 |
| 7 | 0.8667 | 0.8289 | 0.2194 | 0.2817 |
| 8 | 0.7833 | 0.6861 | 0.2838 | 0.418 |
| 9 | 0.8417 | 0.7597 | 0.1819 | 0.3203 |
| 10 | 0.8917 | 0.8667 | 0.1845 | 0.222 |
| 15 | 0.9 | 0.8762 | 0.1748 | 0.2096 |
| 20 | 0.925 | 0.9095 | 0.1687 | 0.1988 |
| 25 | 0.8917 | 0.8597 | 0.1845 | 0.2417 |
| 30 | 0.8583 | 0.8168 | 0.1927 | 0.2519 |
| 35 | 0.8583 | 0.8168 | 0.1927 | 0.2519 |
| 40 | 0.8583 | 0.8168 | 0.1927 | 0.2519 |
| 45 | 0.8583 | 0.8168 | 0.1927 | 0.2519 |
| 50 | 0.8833 | 0.8502 | 0.1532 | 0.1968 |
| 60 | 0.8833 | 0.8476 | 0.1532 | 0.1993 |
| 70 | 0.9083 | 0.8835 | 0.1493 | 0.1904 |
| 80 | 0.8833 | 0.8476 | 0.1532 | 0.1993 |
| 90 | 0.9167 | 0.893 | 0.1361 | 0.1748 |
| 100 | 0.9167 | 0.8905 | 0.1361 | 0.1782 |
| 1944 | 0.8833 | 0.8609 | 0.2194 | 0.2527 |

## Summary stats from testing phase

Table 2: Classification metrics from twenty class-balanced and randomized runs.

| run | Variables | Accuracy | Kappa | AccuracyPValue |
|---|---|---|---|---|
| 1 | 40 | 1 | 1 | 2.216e-07 |
| 2 | 40 | 0.8462 | 0.803 | 9.42e-05 |
| 3 | 1944 | 0.9231 | 0.9008 | 6.703e-06 |
| 4 | 80 | 0.9231 | 0.8992 | 6.703e-06 |
| 5 | 100 | 0.9231 | 0.8992 | 6.703e-06 |
| 6 | 100 | 1 | 1 | 2.216e-07 |
| 7 | 1944 | 1 | 1 | 2.216e-07 |
| 8 | 70 | 1 | 1 | 2.216e-07 |
| 9 | 80 | 1 | 1 | 2.216e-07 |
| 10 | 50 | 1 | 1 | 2.216e-07 |
| 11 | 35 | 1 | 1 | 2.216e-07 |
| 12 | 1944 | 1 | 1 | 2.216e-07 |
| 13 | 1944 | 0.9231 | 0.8992 | 6.703e-06 |
| 14 | 1944 | 0.8462 | 0.7969 | 9.42e-05 |
| 15 | 30 | 1 | 1 | 2.216e-07 |
| **16** | **20** | **1** | **1** | **2.216e-07** |
| 17 | 15 | 0.9231 | 0.9015 | 6.703e-06 |
| 18 | 90 | 0.9231 | 0.9008 | 6.703e-06 |
| 19 | 25 | 1 | 1 | 2.216e-07 |
| 20 | 35 | 0.9231 | 0.9008 | 6.703e-06 |

| Accuracy_Mean | Accuracy_SD | Accuracy_Max |
|---|---|---|
| 0.9577 | 0.05279 | 1 |

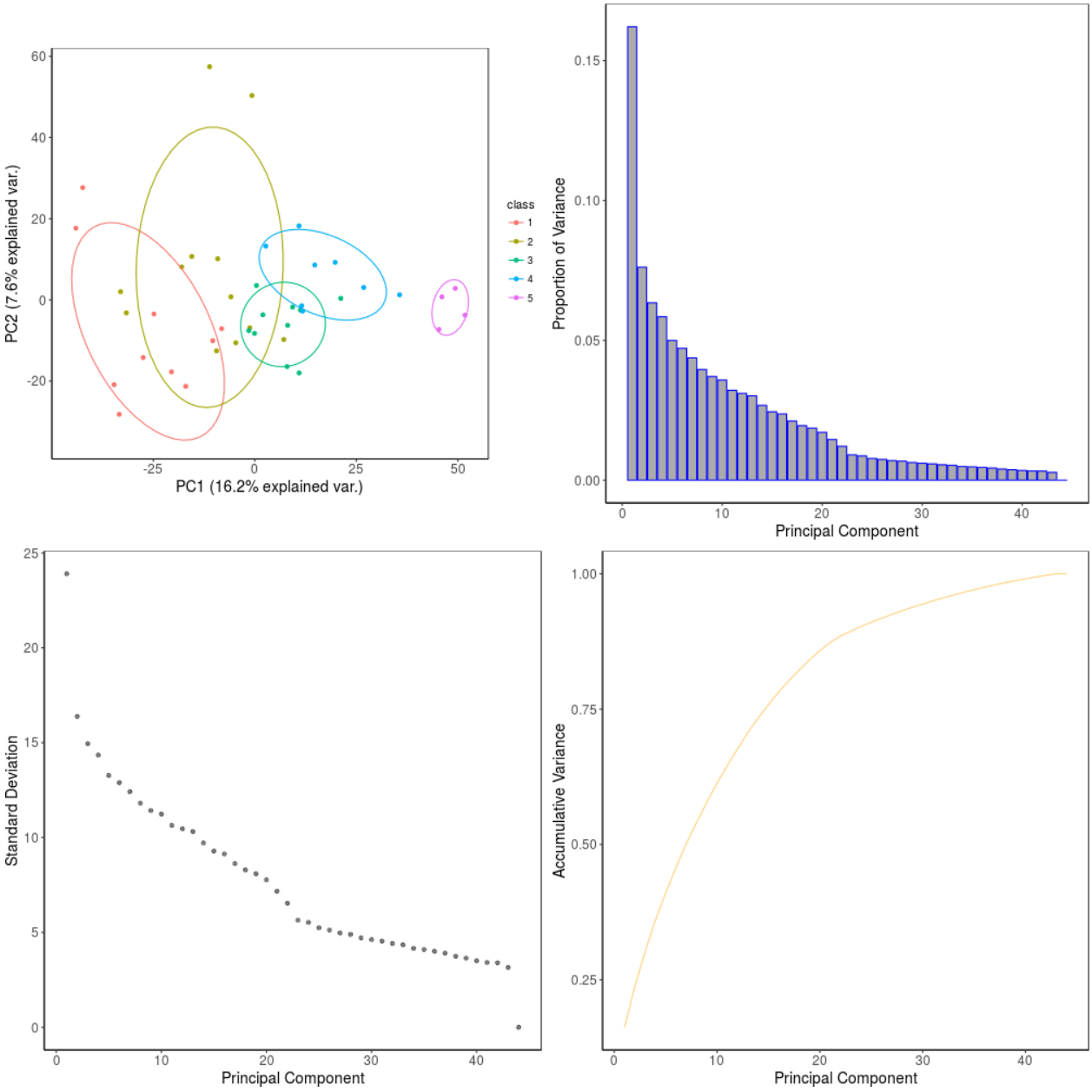
## Workflow runtime

4.983 minutes

# Plots

## Visualization of the classification using PCA

- Groups distribution on the first two Principal Components (PC1 and PC2) from the original data (without apply any FS method).



- Groups distribution on the first two Principal Components (PC1 and PC2) after to apply the FS workflow.