Chemical Sample Classification Report

Petter Lövehagen

2023-05-08

## Brief

The brief is to develop a classification tool to classify chemicals into classes.

In addition, the client is interested in knowing whether all variables are *necessary* for achieving optimal out-of-sample classification performance, or if a subset of measurements will suffice.

This report will aim to:

* explore, analyse and feedback on the provided dataset
* develop an optimised classification model
* determine whether all variables are required
* provide recommendations and options, as applicable

|  |
| --- |
| Note |
| Additional technical details are available in the code comments. |

## Data

The supplied dataset contains 2500 measurements of 20 numerical variables.

The analysis team and report writer did not have any contextual information about the data, e.g.:

* what has been measured
* variable importance, interactions
* measurement scale, units, reliability

Therefore, variables are treated equally and without bias in the analysis and modelling. Decisions are made on statistical grounds and stated assumptions.

|  |
| --- |
| Tip |
| Additional domain-specific information about the data could result in alternative modelling decisions and outcomes and should be considered by the client. |

### Missing data

Before proceeding with [Exploratory Data Analysis](#sec-exploratory-data-analysis), it is important to explore the extent of missing data and whether there are patterns to the missingness. Some classification models assume no missing data, and depending on the amount, prevalence and patterning of missing data, different assumptions and techniques can be applied.

We investigate missingness to see whether the assumption that missing data is ‘missing at random’ (MAR) holds - that is, is the probability of missingness only dependent on **observed** variables? If so and there is a significant amount of missing data (>5%), multiple imputation approaches may be explored to *impute* missing values by estimation through statistical inference.

The sample has 49 rows with at least one missing value, which is 0.09% of the entire dataset. As there are fewer missing values than the 5% threshold, imputation is not required and removing these rows is acceptable.

|  |
| --- |
| Figure 1: Visualised Missing Data |

If the missing data is not MAR - that is, it appears to depend on **unobserved** variables, there may be other, more appropriate imputation methods such as maximum likelihood imputation. Unobserved influences in this scenario may include the sample purity/quality, sample handling/measuring differences, measurement/equipment discrepancies or chemical compositions of the samples.

*Imputation* can introduce bias into the analysis if the assumptions of the imputation method are violated, or the imputed values differ significantly from true missing values.

|  |
| --- |
| Caution |
| The client should consider missingness in their data:   * Are there any concerns regarding missing data? * Is the equipment, staff, technique, facilities, chemicals, etc. consistent? * What are the reasons for missing data? Can they be mitigated? * Can data be collected where it has been identified as missing? * Is there likely to be (more, less, similar amount of) missing data in the future? |

#### Missing value details by class and variable

This dataset has 18 variables with missing data. The five variables with the most missing data are:

| **Variable** | **Count** | **Percentage** |
| --- | --- | --- |
| **X9** | 6 | 0.24 |
| **X18** | 5 | 0.20 |
| **X1** | 4 | 0.16 |
| **X6** | 4 | 0.16 |
| **X15** | 4 | 0.16 |

**Table** **:** Top 5 Variables with missing data, by count

**?(caption)**

Variable X9 has the most missing values with 6, accounting for 0.24% of this variable’s data.

No single sample (observation) has more than 1 missing values. This means that, at most, a sample is missing 4.76% of its data.

The upset plot below shows the five variables with the most missing values and confirms that there are no instances where there are missing values in two variables in the same observations.

|  |
| --- |
| Figure 2: Upset plot of missing data |

If we group missing data by the target label, we see that E has the most missing data at 0.52%.

| **Label** | **Count** | **Percentage** |
| --- | --- | --- |
| **A** | 10 | 0.40 |
| **B** | 6 | 0.24 |
| **C** | 10 | 0.40 |
| **D** | 10 | 0.40 |
| **E** | 13 | 0.52 |

**Table** **:** Missing Data by Class (label)

**?(caption)**

Patterns of missingness begin to emerge when examining missing data for variables, grouping by ‘labels’. It seems that there is a relationship between missing values for sequential variables when grouping observations. This is clearly visible in the heatmap below as well as in the stepped pattern in [Figure 1](#fig-missData) above.

|  |
| --- |
| Figure 3: Heatmap of missing data per variable, grouped by Chemical class |

It is important to note that the target variable (‘label’) has no missing values.

|  |
| --- |
| Warning |
| Is there anything systemic, in terms of missingness:   * X1-X4 is *only* missing for label A * X6, X8 are *only* missing for label B * X9-X12 is *only* missing for label C * X13-X16 are *only* missing for label D * X17-X19 are *only* missing for label E   Is there a relationship between the variables, in terms of what they measure? |

[include citation to missing data references]

|  |
| --- |
| Decision |
| Given the minimal amount of missing data - it will be removed before exploratory data analysis, data splitting and modelling.  If this dataset is representative, the missing data may not be an issue in the future - assuming the pattern identified above is understood. |

### Splitting data

Before proceeding with additional exploratory analysis, we split the dataset into three random subsets:

* train - used to *train* the classification model to *learn* the relationship between the variables and the label
* validation - used to *validate* the performance of the trained model(s) and to tune any hyperparameters; determines how well the model generalises to ‘unseen’ data
* test - used to *evaluate* the final performance of the model post training and tuning; this data is only used once and kept separate.

In order to not introduce bias into the modelling process, the data will be split prior to any EDA, where the dataset is explored and summarised. Any insights or observations made during EDA will emerge solely from the training subset.

The only thing we check in advance is the target variable balance - that is the split across labels. Given that it is not *perfectly* balanced, the data subsets will be split with ‘stratification’ ensuring that each partition has a representative proportion of each class.

| **label** | **Frequency** | **Percent** |
| --- | --- | --- |
| **A** | 508 | 20.73 |
| **B** | 492 | 20.07 |
| **C** | 492 | 20.07 |
| **D** | 487 | 19.87 |
| **E** | 472 | 19.26 |

**Table** **:** Frequency Table by Class (label)

**?(caption)**

|  |
| --- |
| Decision |
| The clean dataset is sufficiently large to split:   * train - 50% * validation - 25% * test - 25% |

[histograms] [outliers] [pair plots] [correlation]

### Exploratory Data Analysis

Throughout EDA and model training, only the train dataset will be analysed. It has 1225 rows, with an overall minimum value of -0.52 (NA) and a maximum value of 16.76 (NA).

The variables have different scales and variances:

| **Statistic** | **Minimum** | **Maximum** |
| --- | --- | --- |
| **Mean** | 0.25 (X8) | 13.8 (X5) |
| **Variance** | 0.04 (X10) | 1.57 (X4) |
| **Range** | 1.42 (X18) | 8.37 (X14) |

**Table** **:** Minimum / Maximum Statistics in 'train'

**?(caption)**

At glance, we can see that there is a significant spread between the variables in terms of mean, variance and range. In order to mitigate against any one variable having undue influence and because nothing is known about the variables, they will be normalised or standardised so that they have the same scale from 0 to 1.

Observations \* many normal distributions \* some which differ across labels, eg. X7-X11

## NOTES BELOW

so there appears to be value in two different approaches \* correlation for dimension reduction \* needs domain knowledge to clarify and ratifiy, explain

* feature reduction - several variables which may be superfluous, measuring similar things or do not add to the model

To do \* normalise and scale \* check for outliers \* address outliers as appropriate \* correlation plot

To try:

interpretation - say what you see \* sparse - lots of variables which are not correlated with each other \* x17-20, and x7-10 appear to correlate, some neg, some pos

### dimension reduction:

PCA - identify principal components, linear combos of original variabes explaining the most variation in the data, plot to see in a lower dimension space t-SNE

PCA:

like a plot with PC1, PC2 the actual 5 classes (shape and label by label) pca arrows and variable labels

(see penguin example)