LWT - Food Science and Technology 184 (2023) 115095

Contents lists available at ScienceDirect

LWT

journal homepage: www.elsevier.com/locate/lwt

# Classification of cheese varieties from Switzerland using machine learning methods: Free volatile carboxylic acids

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A R T I C L E I N F O

*Keywords:*
Cheese
Supervised machine learning
Characterisation
Differentiation
Free volatile carboxylic acids
SHAP value

A B S T R A C T

In the first two decades of the 21st century, a wide range of analyses, including free volatile carboxylic acids (FVCAs), endeavoured to describe 10 different cheese varieties from Switzerland. The aim of the present work was to investigate whether these 10 cheese varieties could be classified by means of supervised machine learning (ML) techniques, as well as to analyse the importance of the features FVCAs in order to understand their role in characterising cheese varieties. Special emphasis was placed on SHAP values (SHapley Additive exPlanations). In total, 241 cheese samples were classified using different ML algorithms with the help of the PyCaret library; at least 90% were correctly classified with two ensemble algorithms: Extra Trees and Random Forest. The fewest misclassifications were observed for Emmentaler AOP, Raclette du Valais AOP, and Formaggio d'Alpe Ticinese DOP, whereas most misclassifications occurred between Le Gruyère AOP and Berner Alpkäse AOP. The most important feature was C1, followed by C3, C6, and iso-C4, with iso-C6 being the least important after C2 and C4. By means of the interpretation of SHAP values applied as a differentiating feature, key FVCAs were identified for most cheese varieties. This study represents a first step towards improved differentiation of cheese varieties.

## 1. Introduction

Approximately 200,000 tonnes of cheese are produced in Switzerland every year, which corresponds to ~45% of the milk produced there (TSM Treuhand, 2021). Cheese production is therefore an economic sector of considerable importance, where a major part of the cheese varieties is produced by local and artisan cheese dairies (Forney & Häberli, 2017; Schmitt, Keech, Maye, Barjolle, & Kirwan, 2016). The territorial associations of these varieties, the long tradition of cheese making, and the high cheese quality were the main reasons for several cheese consortia to apply for an AOP (appellation d'origine protégée), which is a protected designation of origin (FOAG, 2022; Maye, Kirwan, Schmitt, Keech, & Barjolle, 2016; Swiss PDO-PGI Association, 2023). In the year 2000, L'Etivaz was the first cheese in Switzerland to be so registered.

This development increased interest in describing different cheese varieties at different ripening stages by means of a wide range of chemical, biochemical, biological, physical, and sensory analyses. However, most of these projects have been published, if ever, on a national level only. Table 1 summarises the cheese varieties, including references and consortia that have performed an analytical description of each variety. The aims of the individual cheese consortia were primarily to produce descriptive characterisations, but the ideas of classification and differentiation were also a driving force behind these projects. Only a comparison with other cheese varieties can answer the question of how one cheese variety can be distinguished from another (Coker, Crawford, Johnston, Singh, & Creamer, 2005). However, as these characterisations were carried out independently of one another, the goals of classification and differentiation remained unachieved.

In recent years, machine learning (ML) techniques have gained importance, and at the moment, their applications in food safety, processing, quality, and authenticity are increasing almost exponentially (Jimenez-Carvelo, Gonzalez-Casado, Bagur-Gonzalez, & Cuadros-Rodriguez, 2019; Khan, Sablani, Nayak, & Gu, 2022; Wang, Bouzembrak, Lansink, & van der Fels-Klerx, 2022). ML is a branch of artificial intelligence that enables algorithms to learn continuously and improve upon (past) data and make predictions based on them (Alzubi, Nayyar, & Kumar, 2018). If the data are labelled, classification – a supervised ML technique – is additionally possible. This task requires the algorithms to learn how a label should be assigned to the data – in our case, determining cheese varieties from the analysed parameters, the so-called features. Depending on the underlying algorithm, ML techniques can be grouped into classical (also called 'conventional') or deep

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https://doi.org/10.1016/j.lwt.2023.115095
Received 24 April 2023; Received in revised form 6 July 2023; Accepted 15 July 2023
Available online 15 July 2023

**Glossary**

| | |
|---|---|
| FVCA | free volatile carboxylic acid |
| C1 | formic acid |
| C2 | acetic acid |
| C3 | propionic acid |
| C4 | butyric acid |
| iso-C4 | isobutyric acid, 2-methylpropionic acid |
| iso-C5 | isovaleric acid, 3-methylbutyric acid |
| iso-C6 | isocaproic acid, 4-methylpentanoic acid |
| SHAP | SHapley Additive exPlanations |
| GC | gas chromatograph |
| ML | machine learning |
| AOP | appellation d'origine protégée |
| RF | Random Forest classifier |
| ET | Extra Trees classifier |
| LR | Linear Regression classifier |
| LightGBM | Light Gradient Boosting Machine |

learning, each supervised or unsupervised (LeCun, Bengio, & Hinton, 2015). Classical supervised ML algorithms are preferably used when dealing with analytical data (Koren et al., 2020; Magnus, Virte, Thienpont, & Smeesters, 2021; Pérez-Rodríguez, Gaiad, Hidalgo, Avanza, & Pellerano, 2019; Wang et al., 2022). Supervised ML methods applied to measurements made on a chemical system are often called 'chemometrics' (Jimenez-Carvelo et al., 2019). Examples of chemometric classifications in food science can be found in several studies (Cocchi, Biancolillo, & Marini, 2018; de Andrade et al., 2022; Di Donato, Biancolillo, Mazzulli, Rossi, & D'Archivio, 2021). One strength of such an approach for the current study is the possibility of interpreting the results post hoc, using SHapley Additive exPlanations values (SHAP; see section 2.3), whereas deep learning does not allow a look 'behind the scenes'. The application of deep learning classification algorithms in food production is mostly used in image analysis (Arslan, Memis, Sonmez, & Batur, 2022; Loddo, Di Ruberto, Armano, & Manconi, 2022; McAllister, Zheng, Bond, & Moorhead, 2018).

Traditional cheese classification systems are usually based on milk type, milk treatment, coagulation methods, textural properties, and/or specific ripening patterns, all in combination with compositional data (Almena-Aliste & Mietton, 2014). To the best of our knowledge, a supervised ML approach to classifying different cheese varieties on the basis of compositional data has not yet been published. However, it should not be disregarded that chemometric classification studies on cheese have already been performed, although with a different focus. Barile, Coïsson, Arlorio, and Rinaldi (2006) applied a neural network to predict Ossolano cheese production origin in order to guarantee the authenticity of this PDO cheese. Similarly, Brazilian artisanal cheeses were analysed for their mineral content and divided into production areas (de Andrade et al., 2022). The authors were able to classify the analysed cheeses with supervised ML methods (Random Forest (RF) and Support Vector Machines), reaching accuracy and kappa scores of >0.8. Di Donato et al. (2021) also used supervised ML methods to discriminate between Italian PDO Pecorino cheeses by their volatile fractions. They were able to reach an accuracy score for correct classification of 0.875 with linear and partial least squares discriminant analyses.

Finally, in the 1980s, Aishima and Nakai (1987) applied stepwise discriminant analysis to gas chromatograph (GC) profiles to classify cheese varieties (Cheddar, Gouda, Edam, Swiss, and Parmesan). Discriminating between Gouda and Edam revealed itself to be the most difficult. In cheeses from Switzerland, free volatile carboxylic acids (FVCAs) C1–C6 are often determined for quality assessment reasons, as they were for all the studied cheese varieties listed in Table 1. FVCAs are always formed during cheese ripening as metabolites from the fermentation of pentoses, hexoses, and lactate by starter, non-starter, or secondary cultures (C1–C4), from the hydrolysis of milk fat (C4, C6), or from amino acid catabolism (iso-C4–iso-C6) (Badertscher, Blaser, & Noth, 2023). Most of these FVCAs – except for C1 – may also be produced by lactococci, lactobacilli, and/or surface microbiota from amino acids after carbohydrate starvation (Ganesan, Seefeldt, & Weimer, 2004; Ganesan & Weimer, 2017). For simplicity's sake, the FVCAs will be divided into the three groups described above. FVCAs probably contribute to the typical flavour of all known cheese varieties (McSweeney, Fox, Cotter, & Everett, 2017).

As can be seen in Table 1, most of these data were collected and filed in the first 20 years of the 21st century. In the present work, these data shall be brought together with the aim of answering the following questions, irrespective of the maturity stage:

- Can cheese varieties be classified by their FVCA profiles using supervised ML methods?
- Which features from the FVCA profile are important for classification? Could they be used to differentiate one variety from another?

**Table 1**
Cheese varieties from Switzerland that have been analytically characterised (*N* = number of samples/observations). AOP, appellation d'origine protégée; DOP, denominazione di origine protetta.

| Cheese variety | *N* | Link to consortia | References |
|---|---|---|---|
| **Appenzeller®** [a] | 29 | www.appenzeller.ch | Fröhlich-Wyder, Beutler, Bütikofer, Lavanchy, and Winkler (2003) |
| **Berner Alpkäse AOP** | 10 | www.casalp.ch | Jakob, Badertscher, and Bütikofer (2007) |
| **Berner Alpkäse AOP** [a] | 26 | www.casalp.ch | Jakob and Piccinali (2010) |
| **Berner Hobelkäse AOP** | 10 | www.casalp.ch | Jakob et al. (2007) |
| **Emmentaler AOP** [a, b] | 58 | www.emmentaler.ch | Wyder, Bosset, Casey, Isolini, and Sollberger (2001) |
| **L'Etivaz AOP** | 10 | www.etivaz-aop.ch | Goy and Wechsler (2015) |
| **L'Etivaz à rebibes AOP** | 7 | www.etivaz-aop.ch | Goy and Wechsler (2015) |
| **Formaggio d'Alpe Ticinese DOP** [a] | 16 | www.formaggio-alpe-ticino.ch | Haldemann (2010) |
| **Le Gruyère AOP** [a] | 30 | www.gruyere.com | Fröhlich-Wyder, Goy, Häni, Lavanchy, and Bosset (2003); Lavanchy, Bütikofer, Häni, Goy, and Fröhlich-Wyder (2002) |
| **Le Gruyère AOP** [a] | 18 | www.gruyere.com | Goy, Piccinali, Wechsler, and Jakob (2011) |
| **Raclette du Valais AOP** | 21 | www.raclette-du-valais.ch | Wechsler et al. (2021) |
| **Sbrinz AOP** [c] | 28 | www.sbrinz.ch | Eugster, Berthoud, and Amrein (2011) |

[a] Different maturity stages.
[b] At that time, Emmentaler did not hold an AOP yet. Two different cultures of *P. freudenreichii* were used.
[c] Cheeses were analysed within the framework of a trial in Sbrinz cheese factories. Different NSLAB cultures were tested.

## 2. Materials and methods

### 2.1. Information on the cheese varieties (the target)

The targets are typical cheese varieties from Switzerland that are more or less well known depending on the region. They are listed in Table 1 with corresponding references and websites where more information on the individual varieties can be found. With the exception of Appenzeller®, all of the cheeses are registered as AOP (PDO and DOP in English and Italian, respectively) with the Swiss Federal Office for Agriculture (FOAG, 2022). They are all produced from raw milk and have different maturity stages, depending on the variety and on the preferred ripeness at the time of consumption. The youngest cheeses are the semi-hard varieties Appenzeller®, Formaggio d'Alpe Tincinese DOP, and Raclette du Valais AOP, aged 3–6 months, and the oldest cheeses are found among the extra-hard cheese varieties Berner Hobelkäse AOP, L'Etivaz à rebibes AOP, and Sbrinz AOP, aged 25–35 months. All three varieties are often eaten as shaved cheese. Le Gruyère AOP, Emmentaler AOP, and Berner Alpkäse AOP are ripened for 3–13 months. All cheese samples were judged by the respective consortia to be of good quality.

For simplicity's sake, the term AOP will be omitted throughout the following text.

### 2.2. Data preparation: From the raw data to the working data

As described above, several cheese varieties from Switzerland were characterised by means of various analyses, such as their GC profiles (C1–C6). The FVCAs were determined according to the method described by Fröhlich-Wyder et al. (2013). '20 g of cheese was first distilled in an acidic medium with steam and the distillate titrated with NaOH to determine the total acidity. Subsequently, 1 mL of the over-titrated solution was esterified and the relative concentrations of each FVCA were determined by headspace injection on a GC-FID. Together with the total acidity, the individual absolute contents could then be calculated' (Badertscher et al., 2023). Information on sampling can be found in the references listed in Table 1. In most cases, a piece of 2–3 kg of cheese had been provided by the consortia. At least 0.5 cm of the rind of the smear-ripened cheeses had been removed and at least 3 cm of the hoop side. The remaining cheese had been grated and mixed before analysis.

The raw data extracted from the database included 241 observations (cheese samples), eight features (FVCA), and one categorical variable, the target (cheese variety). The raw dataset had no missing data, which is important for classification. Furthermore, the sum of FVCAs was not included in the analysis since it strongly correlated with acetic (C2, $r = .985$) and propionic (C3, $r = .990$) acids. However, looking at the individual cheese groups, C2 correlated strongly with total FVCAs in most cheese varieties (except for Berner Hobelkäse and L'Etivaz à ribibes) but not C3, which only highly correlated with total FVCAs in Emmentaler and L'Etivaz (results not shown).

Cheese is a natural product; therefore, variations must be expected in FVCA content. For this reason, a purely mathematical definition of outliers, such as the 1.5 × IQR rule, is not useful and would lead to the elimination of too many observations. It was thus decided to keep all samples in the dataset.

The final dataset, the working file, consists of 241 observations, eight features, and the target cheese variety.

### 2.3. The modelling process

Fig. 1 shows the most important steps for classification with ML methods. Since classification is a supervised learning process (i.e., the target variables are known), the algorithms must be provided with a dataset to train a model. Training was conducted with 70% of the data (168 randomly selected samples), which were additionally split into 10 equally sized subsets for cross-validation. Using the trained model, predictions were then generated with the remaining test data (the remaining 30%, i.e. 73 samples). A comparison of the predictions with

**Table 2**
Classifiers used in the present study (PyCaret).

| ID | name | reference |
|---|---|---|
| **LR** | logistic regression | sklearn.linear_model._logistic.LogisticRegression |
| **KNN** | k-nearest neighbors classifier | sklearn.neighbors._classification.KNeighborsClassifier |
| **NB** | naive Bayes | sklearn.naive_bayes.GaussianNB |
| **DT** | decision tree classifier | sklearn.tree._classes.DecisionTreeClassifier |
| **SVM** | SVM – linear kernel | sklearn.linear_model._stochastic_gradient.SGDClassifier |
| **Ridge** | Ridge classifier | sklearn.linear_model._ridge.RidgeClassifier |
| **RF** | Random Forest classifier | sklearn.ensemble._forest.RandomForestClassifier |
| **QDA** | quadratic discriminant analysis | sklearn.discriminant_analysis.QuadraticDiscriminantAnalysis |
| **ADA** | AdaBoost classifier | sklearn.ensemble._weight_boosting.AdaBoostClassifier |
| **GBC** | gradient boosting classifier | sklearn.ensemble._gb.GradientBoostingClassifier |
| **LDA** | linear discriminant analysis | sklearn.discriminant_analysis.LinearDiscriminantAnalysis |
| **ET** | Extra Trees classifier | sklearn.ensemble._forest.ExtraTreesClassifier |
| **LightGBM** | Light Gradient Boosting Machine | lightgbm.sklearn.LGBMClassifier |
| **Dummy** | dummy classifier | sklearn.dummy.DummyClassifier |

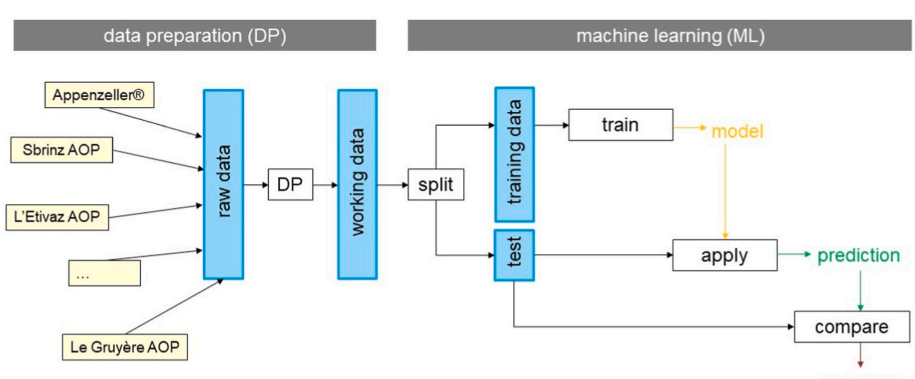


**Fig. 1.** Representation of a typical machine learning process.

the true values enables a quality assessment of the model by calculating the accuracy scores.

The modelling process was carried out with the open-source low-code machine learning library PyCaret (Ali, 2020). It supports numerous ML algorithms; 14 classifiers were tested in this work, which are listed in Table 2, including their references. PyCaret applies the above-described train-eval-testing validation technique. The output of the model comparison is a table with the average scores of all models across the folds (10) and with the required times. The classification metrics in the output are accuracy, area under the curve (AUC), recall, precision, F1, Cohen's kappa, and the Matthews correlation coefficient (MCC). These metrics represent always specified count fractions; this is why they are often indicated in %. The library also helps in pre-processing (e.g., it standardises and deals with imbalanced data, tunes the hyperparameters, and may even take over the feature engineering task). Since there were only eight features which had been investigated, the feature selection task was omitted. The following parameters were chosen in the setup function: *remove_outliers = False, transformation = True, normalize = True, normalize_method = 'robust'*. Fine-tuning the best model did not improve the results.

### 2.4. Model interpretation

In order to understand the significance of each feature for the classification of the cheese varieties, the feature importance of the tree-based models was extracted, and the according SHAP values (SHapley Additive exPlanations) were calculated with the SHAP module in Python (Lundberg, 2018). The latter assigns each feature of each cheese variety an importance value (Lundberg & Lee, 2017); it uses the classic Shapley values from game theory. The SHAP values help to interpret the classifications and, therefore, could be a valuable tool to differentiate cheese varieties.

## 3. Results and discussion

### 3.1. Data exploration

Fig. 2 shows the distribution of the observations (samples) for each cheese variety. As can be seen, there are several outliers present across nearly all the cheese varieties and FVCAs. The outliers are found in the upper part of the boxplots, indicating a right- or positive-skewed distribution. In fact, skewness calculated for the distributions shows that the majority of the values are positive (results not shown). The negative values reached a negative maximum of −0.283, indicating a fairly normal distribution; this was the case for C1, C2, C6, and iso-C4. The maximal positive values (>4.5) were found for iso-C4 and iso-C5 in Sbrinz, because only one and seven observations, respectively, contained these FVCAs; they were missing in all the other samples. This explains the strongly right-skewed distribution. A similar observation was conducted for iso-C6 in Le Gruyère. Also, higher values were calculated for C3, with the exception of the varieties L'Etivaz à rebibes and Emmentaler. The only relevant source of C3 in cheese is *Propionibacterium freudenreichii*. These bacteria naturally occur in raw milk as wild strains (Turgay et al., 2011), can grow during maturation, and produce a varying amount of C3 in a strain-dependent manner but mainly contingent upon their ability to grow to higher concentrations. In the case of Emmentaler, the only Swiss-type cheese in this study, *P. freudenreichii* is deliberately added as a culture during production in order to obtain the characteristic eyes and a relevant amount of C3 (Fröhlich-Wyder et al., 2022). Due to this fact, the final concentrations of *P. freudenreichii* in mature Emmentaler are within the same order of magnitude for all samples, allowing C3 levels to occur at a near-normal distribution. L'Etivaz à rebibes is a long-ripened and high-cooked cheese with a high salt content; this combination inhibits the growth of propionic acid bacteria. Therefore, the right-skewed distribution of C3 in the other cheese varieties is due to naturally occurring outliers. The remaining FVCAs reached values of 2–3, also indicating right-skewed distributions. This is easily recognisable from the medians being often situated in the lower part of the boxes (Fig. 2). Right-skewed

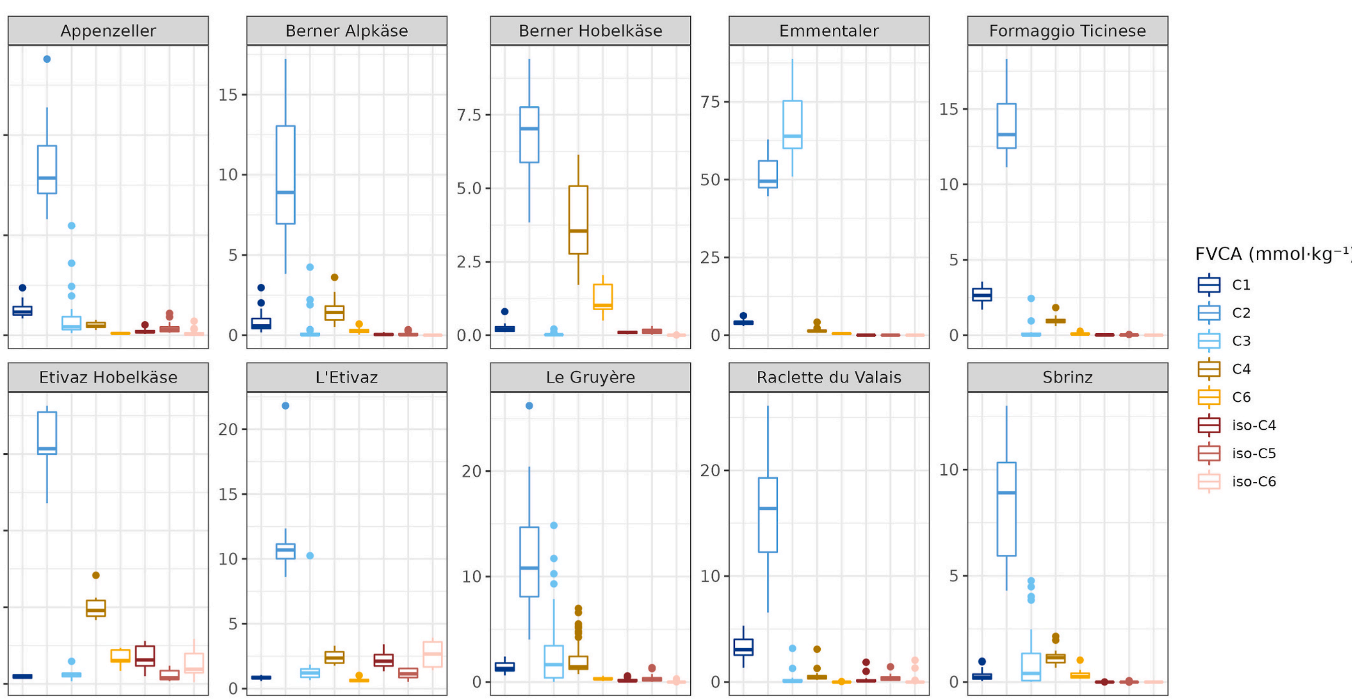


**Fig. 2.** Boxplots of FVCAs grouped by cheese variety. The number of observations can be found in Table 1. The y-scale is adapted to the FVCA range of each cheese variety. (FVCA, free volatile carboxylic acids; C1, formic acid; C2, acetic acid; C3, propionic acid; C4, butyric acid; iso-C4; isobutyric acid; iso-C5, isovaleric acid; iso-C6, isocaproic acid).

**Table 3**
Performance results of a model training session in PyCaret (mean of 10 runs with 70% of the data).

| Model | Accuracy | AUC | Recall | Prec. | F1 | Kappa | MCC | TT (s) |
|---|---|---|---|---|---|---|---|---|
| **ET** | 0.9346 [a] | 0.2000 | 0.9279 | 0.9352 | 0.9259 | 0.9241 | 0.9279 | 0.3180 |
| **LR** | 0.9107 [b] | 0.1992 | 0.9261 | 0.9350 | 0.9038 | 0.8967 | 0.9036 | 0.0310 |
| **RF** | 0.9103 [c] | 0.2000 | 0.8886 | 0.9104 | 0.9012 | 0.8960 | 0.9003 | 0.3110 |
| **LightGBM** | 0.9040 [d] | 0.1992 | 0.8700 | 0.9088 | 0.8906 | 0.8891 | 0.8960 | 0.0720 |
| **KNN** | 0.8809 | 0.1953 | 0.8750 | 0.9057 | 0.8729 | 0.8625 | 0.8695 | 0.0920 |
| **LDA** | 0.8743 | 0.1992 | 0.8751 | 0.9003 | 0.8660 | 0.8550 | 0.8625 | 0.0080 |
| **NB** | 0.8507 | 0.1949 | 0.8386 | 0.8571 | 0.8306 | 0.8269 | 0.8382 | 0.0110 |
| **GBC** | 0.8504 | 0.2000 | 0.8421 | 0.8502 | 0.8343 | 0.8270 | 0.8362 | 0.4370 |
| **SVM** | 0.8096 | 0.0000 | 0.7956 | 0.8294 | 0.7903 | 0.7792 | 0.7954 | 0.0500 |
| **DT** | 0.7974 | 0.1766 | 0.7772 | 0.7993 | 0.7775 | 0.7670 | 0.7782 | 0.0100 |
| **Ridge** | 0.7081 | 0.0000 | 0.6210 | 0.6191 | 0.6436 | 0.6585 | 0.6742 | 0.0090 |
| **ADA** | 0.3743 | 0.1374 | 0.2924 | 0.2324 | 0.2611 | 0.2505 | 0.3600 | 0.0540 |
| **Dummy** | 0.1787 | 0.1000 | 0.1131 | 0.0319 | 0.0542 | 0.0000 | 0.0000 | 0.0090 |
| **QDA** | 0.1493 | 0.0000 | 0.1131 | 0.0233 | 0.0401 | 0.0000 | 0.0000 | 0.0120 |

[a] *SD*: 0.0488, median: 0.9412.
[b] *SD*: 0.0477, median: 0.8824.
[c] *SD*: 0.0559, median: 0.9100.
[d] *SD*: 0.0494, median: 0.8824.

distributions will always be encountered in the case of cheese production; this is why it was decided to include all outliers in the modelling.

### 3.2. Classification of cheese varieties

Table 3 presents the classification results of the training dataset (mean values of 10 runs). Tree-based classifiers are the most common among the best models, namely the Extra Trees classifier (ET) and Random Forest classifier, two very similar ensemble classifiers (Ceballos, 2019). In the training phase, the two algorithms were able to classify over 90% of the holdout cheese samples correctly. The recall (sensitivity) of the samples was ~4% higher with ET and the precision (reliability) ~2%. Similarly, the F1-score – the harmonic mean of precision and recall – was found to be over 90% for ET. This score is a better accuracy score for imbalanced data than the classical accuracy score, which describes correctly predicted samples. In the present work, as can be seen in Table 1, the data are fairly imbalanced. However, the two scores are similar. The kappa metric describes the agreement between the predicted and true values for cross-validation during training. A better metric for imbalanced data and multiclass issues is the MCC, which calculates the correlation coefficient between the predicted and the true classes. However, all these metrics confirm that ET performed best, although RF, LR (logistic regression), and also the Light Gradient Boosting Machine (LightGBM) – a boosting framework using tree-based algorithms – are very close (Table 3).

As Table 4 shows, >90% of the test data – corresponding to >65 of the 73 test samples – were predicted correctly with the above trained ET and RF algorithms, versus 85% with LightGBM and only 80% with LR. All the other metrics fell within a similar range, with kappa and MCC being somewhat lower than the classical accuracy scores. LR yielded the poorest results for all metrics except recall, which was higher than recall of LightGBM. This is not surprising, even though LR was judged second best during training: the median of the accuracy score showed a large divergence from the mean value, indicating the instability of the algorithm (Table 3).

Table 5 compares the true results with the predicted results for the test data using the trained models. They include misclassifications, which had to be expected because of the similarity of the cheese varieties. As an example, L'Etivaz à rebibes and Berner Hobelkäse are long-ripened variants of L'Etivaz and Berner Alpkäse, respectively (Goy & Wechsler, 2015; Jakob, Badertscher, & Bütikofer, 2007). Other misclassifications – especially those concerning Berner Alpkäse – probably have to do with the high variability of the product (Jakob et al., 2007). Interestingly, Berner Alpkäse is often misclassified as Le Gruyère and vice versa; both are smear-ripened hard cheese varieties that use back-slopping cultures. The fewest misclassifications were observed for Emmentaler, Raclette du Valais, and Formaggio d'Alpe Ticinese.

### 3.3. Feature importance

In tree-based models, the features used as a decision node and contributing to the decrease in splitting impurity are ranked. This ranking can be used to assess the relative importance of these features (Pedregosa et al., 2011), which, in turn, helps in analysing and understanding which features are relevant for the correct classification of cheese varieties. Therefore, those yielded by the top three tree-based classifiers, ET, RF, and LightGBM, were compared (Table 6). All three models agree on the most (or second most) and least important features: C1 was judged to be the most (or second most) important and preferably used as a decision node, while iso-C6 was the least important. C1 is a product originating from the fermentation of citrate by facultatively heterofermentative lactobacilli (FHL), either from the raw milk or an adjunct culture, depending on the cheese variety. C1 is already formed in small quantities during lactic acid fermentation by *Streptococcus thermophilus*, which promotes the multiplication of lactobacilli (Horiuchi & Sasaki, 2012; Yamamoto, Watanabe, Ichimura, Ishida, & Kimura, 2021). Appenzeller®, Emmentaler, and Formaggio d'Alpe Ticinese are produced with an adjunct culture of FHL; Raclette du Valais has a high prevalence of FHL originating from the raw milk, as shown by microbiome analysis (Wechsler et al., 2021). This is why they contain higher levels of C1 compared to the other cheese varieties (see references in Table 1). On the other hand, the extra-hard cheeses Sbrinz, Berner Hobelkäse, and L'Etivaz à rebibes, with high cooking temperatures of >50 °C, contain very low amounts of C1 as a consequence of the

**Table 4**
Performance results of the top four models in PyCaret (with remaining 30% of the data, the test data).

| Model | Accuracy | AUC | Recall | Prec. | F1 | Kappa | MCC |
|---|---|---|---|---|---|---|---|
| **ET** | 0.9315 | 0.9874 | 0.9374 | 0.9356 | 0.9314 | 0.9204 | 0.9208 |
| **LR** | 0.8082 | 0.9764 | 0.8622 | 0.8455 | 0.8139 | 0.7790 | 0.7843 |
| **RF** | 0.9178 | 0.9945 | 0.9318 | 0.9260 | 0.9187 | 0.9046 | 0.9056 |
| **LightGBM** | 0.8493 | 0.9867 | 0.7658 | 0.8542 | 0.8442 | 0.8241 | 0.8247 |

**Table 5**
Cross table of the true values (columns) and the predicted values (rows) from the top three tree-based models obtained from the modelling process in PyCaret (ET, RF, LightGBM). Example for Le Gruyère: *With ET, 16 out of the 17 samples in the test set had been classified correctly and one sample had been misclassified as Berner Alpkäse.*

| | Appenzeller | Berner Alpkäse | Berner Hobelkäse | Emmentaler | L'Etivaz | L'Etivaz à rebibes | Formaggio d'Alpe Ticinese | Le Gruyère | Raclette du Valais | Sbrinz |
|---|---|---|---|---|---|---|---|---|---|---|
| Appenzeller | 4, 4, 4 | | | | | | | | | |
| Berner Alpkäse | | 9, 9, 8 | | | | | | 1, 1, 2 | | 1, 1, 1 |
| Berner Hobelkäse | | 1, 1, 2 | 2, 2, 1 | | | | | | | |
| Emmentaler | | | | 10, 10, 10 | | | | | | |
| L'Etivaz | | | | | 3, 3, 1 | | | 0, 0, 1 | | |
| L'Etivaz à rebibes | | | 0, 0, 1 | | | 2, 2, 1 | | | | |
| Formaggio d'Alpe Ticinese | | | | | | | 6, 6, 6 | | | |
| Le Gruyère | 0, 0, 1 | 2, 3, 1 | | | | | | 16, 15, 16 | | |
| Raclette du Valais | | | | | | | | | 8, 8, 8 | |
| Sbrinz | | | | | | | | | | 8, 8, 7 |

**Table 6**
Ranking of the features according to the attribute 'feature importance' of the three top tree-based models (see Table 3), in descending order of importance. 'Feature importance' is a return parameter of all tree-based models.

| ET | RF | LightGBM |
|---|---|---|
| C1 | C1 | C6 |
| iso-C4 | C3 | C1 |
| C3 | iso-C4 | C3 |
| C6 | iso-C5 | iso-C4 |
| iso-C5 | C6 | C4 |
| C2 | C2 | C2 |
| C4 | C4 | iso-C5 |
| iso-C6 | iso-C6 | iso-C6 |

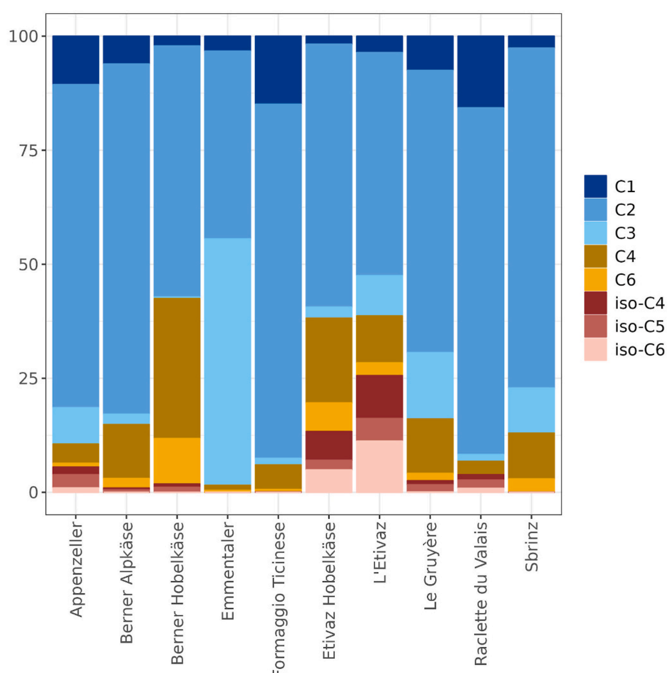


**Fig. 3.** Stacked bar chart of the mean molar FVCA fraction (mol%) grouped by cheese variety. The number of observations can be found in Table 1. Colours represent the main origins; blue: fermentation; yellow: lipolysis; red; proteolysis. (FVCA, free volatile carboxylic acids; C1, formic acid; C2, acetic acid; C3, propionic acid; C4, butyric acid; iso-C4; isobutyric acid; iso-C5, isovaleric acid; iso-C6, isocaproic acid).

inhibition of FHL from the raw milk.

The FVCAs C3, iso-C4, and C6 were among the next most important features; however, the order of their importance was different for each model. C3 is a very specific FVCA originating mainly from propionic acid fermentation, as outlined in section 3.1. Emmentaler contains very high amounts of C3 (>60 mmol kg-1); all the other cheese varieties contain much lower amounts (Figs. 2 and 3). The branched-chain fatty acid iso-C4 is a product of the catabolism of the branched-chain amino acid valine. Aspartic acid, glutamic acid, methionine, and serine can also be precursors of iso-C4, depending on the microbiota present in cheese (Ganesan & Weimer, 2017). The Appenzeller® and both Etivaz varieties contain the most branched-chain fatty acids. They seem to be a distinctive feature of the Etivaz cheese varieties, as Fig. 3 shows. In contrast, C6 is a typical product of lipolysis and is primarily found in long-ripened cheeses, such as Berner Hobelkäse and L'Etivaz à rebibes (Figs. 2 and 3). LightGBM judged C6 to be the most important feature for classification. C2 and C4 are of rather low importance; the reason for the low importance of C4 lies in its high variance, whereas the high prevalence of C2 in all the cheese varieties renders this FVCA less important. The high variance of C4 is due to its two likeliest origins, namely clostridia and lipolysis. Clostridia are considered highly undesirable contaminants but may still be present in very low concentrations in cheeses that form low and changing amounts of C4, whereas lipolysis is dependent on milk quality and is influenced, among others, by feeding and animal breed (Arias-Roth et al., 2022). C2 is formed in many different processes and therefore reaches high concentrations in all the cheeses. In Emmentaler cheeses, it may originate from a specific pathway – propionic acid fermentation – where C2 is produced in parallel to C3 (Fröhlich-Wyder et al., 2022). Finally, the role of iso-C5 seems to be ambiguous, as is the role of iso-C6, an FVCA present in very few cheese varieties if at all, and therefore unimportant for classification.

### 3.4. SHAP values

In order to understand the contribution of each feature to the prediction of every cheese variety, the SHAP values were calculated based on the top three tree-based models (i.e., ET, RF, and LightGBM). The results for the relative mean SHAP values are shown in Fig. 4. The values from the ET and RF models are similar, which is not surprising since they are very close ensemble methods. LightGBM is a boosting method that seems to increase the values of the most important features (e.g., iso-C4 in both Etivaz varieties and Sbrinz). The role of the features will be discussed separately for each variety.

Appenzeller® is a semi-hard, smear-ripened cheese made with an adjunct culture of FHL. This is why C1 is an important characterising feature of this cheese. Furthermore, the iso-FVCAs seem to be important features, indicating the impact of smear ripening on proteolysis, where the microbiota catabolise branched-chain amino acids into the corresponding FVCA (Williams, Beattie, & Banks, 2004). LightGBM increases

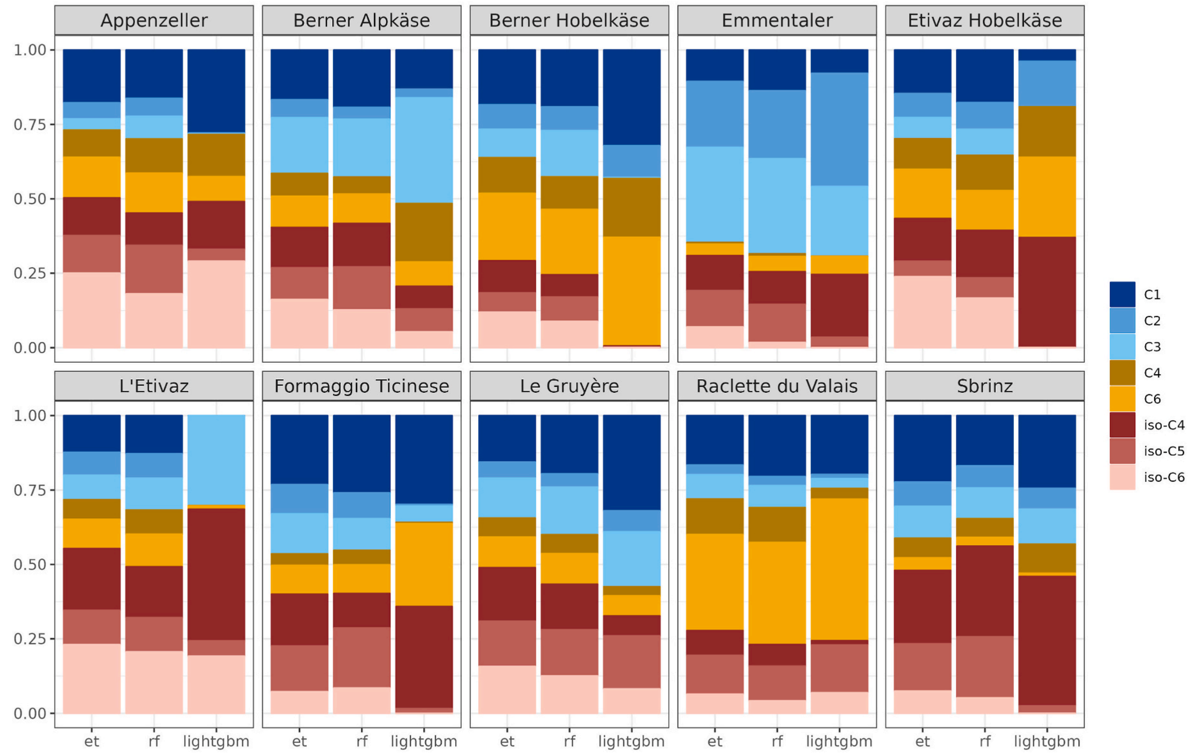


**Fig. 4.** Relative mean SHAP values from the top three tree-based models for each FVCA grouped by cheese variety. The number of observations can be found in Table 1. (SHAP, SHapley Additive exPlanations; FVCA, free volatile carboxylic acids; C1, formic acid; C2, acetic acid; C3, propionic acid; C4, butyric acid; iso-C4; isobutyric acid; iso-C5, isovaleric acid; iso-C6, isocaproic acid).

the SHAP value of C1, confirming its importance in Appenzeller®.

Berner Alpkäse and Berner Hobelkäse are both hard, smear-ripened cheeses produced in the Bernese Alps. For the correct classification of Berner Alpkäse, the presence of low amounts of both C3 and iso-FVCAs plays a major role. Berner Hobelkäse is a long- and dry-ripened Berner Alpkäse which can be eaten as shaved cheese. An important feature for Berner Hobelkäse is the contribution of lipolysis to the FVCAs as a result of the long ripening time (Figs. 3 and 4).

As could be expected, the high content of C2 and C3 is typical of Emmentaler. It is worth noting that iso-C4 and iso-C5 accounted for approximately 25% of the SHAP value, even though these acids had not been determined (Figs. 2 and 3). It can be concluded that the absence of these acids contributes to the correct classification of Emmentaler. The cheese variety is dry ripened; thus, no surface microbiota can influence the catabolism of branched-chain amino acids.

Similar to the Berner Alpkäse and Berner Hobelkäse, the extra-hard L'Etivaz à rebibes is a long-ripened L'Etivaz (hard cheese). As already observed for Berner Hobelkäse, the contribution of lipolysis to the FVCAs in L'Etivaz à rebibes is of importance, but so is the presence of iso-C4. Compared to the other cheese varieties, the Etivaz cheeses show high proportions of iso-FVCAs, which seem to be important for classification: they account for up to 70% of the SHAP value of L'Etivaz. In contrast to Berner Alpkäse and Berner Hobelkäse, the smear-ripening is performed at significantly higher relative humidity in common central ripening rooms (FOAG, 2022), which explains the stronger impact of the smear on these acids. Furthermore, a certain amount of C3, probably originating from propionic acid fermentation, also plays an important role in classification. Although propionic acid fermentation is primarily desirable in Swiss-type cheeses, such as Emmentaler, C3 is found to be typical in L'Etivaz. This is not surprising since it is a variety produced from raw milk, which often contains Propionibacteria to some degree. Surprisingly, C3 is not abundant in Berner Alpkäse, which seems to be characteristic of this variety (Fig. 4).

Formaggio d'Alpe Ticinese is a semi-hard cheese with a natural rind with ubiquitous moulds. The formation of C1 by FHL and the absence of significant quantities of the iso-FVCAs as a result of the absence of smear-ripening was found to be a typical combination for this cheese variety (Figs. 3 and 4).

The hard cheese variety Le Gruyère, also a smear-ripened cheese, has a similar pattern to Berner Alpkäse. In fact, the models misclassified these two cheese varieties repeatedly (Table 5). Interestingly, smearing, much more prevalent in Le Gruyère than in Berner Alpkäse, did not have a strong enough effect on the FVCA pattern to guarantee correct classification. These are the only varieties in this study which are produced with back-slopping cultures.

Raclette du Valais is a smear-ripened semi-hard cheese. Besides C1 and, to a lesser degree, iso-FVCAs, C6 was shown to have the largest SHAP value for this variety. As is evident in Fig. 3, it is the absence of C6, and therefore of lipolysis, which seems to be unique for Raclette du Valais.

Finally, the extra-hard, dry-ripened cheese Sbrinz is differentiated from other cheese varieties by a strong contribution of iso-C4 to a correct classification: its SHAP value was the highest. Similar to Emmentaler, Sbrinz is primarily characterised by the absence of iso-FVCAs but also by low amounts of C1.

## 4. Conclusion

In the present work, 241 samples of 10 different cheese varieties from Switzerland were classified with different ML algorithms on the basis of their FVCA profiles. It was possible to classify 90% of the samples correctly with two ensemble algorithms, ET and RF. The third-best algorithm, LightGBM, was able to classify 84% of the test data correctly. The fewest misclassifications were observed for Emmentaler, Raclette du Valais, and Formaggio d'Alpe Ticinese, whereas most misclassifications occurred between Le Gruyère and Berner Alpkäse. The analysis of the feature importance attributes revealed that C1 was the most important feature, followed by C3, C6, and iso-C4. In order to

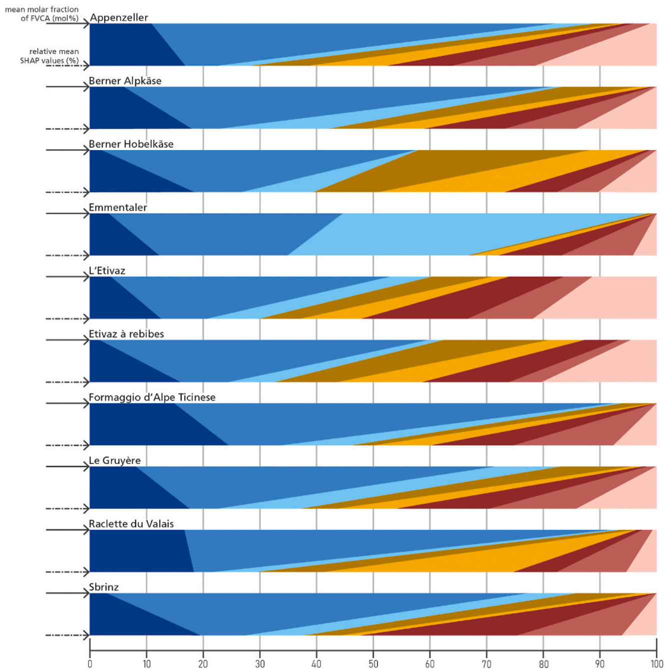


**Fig. 5.** Mean molar FVCA fraction represented by the upper edge (⟶ mol%) and relative mean SHAP values from the top two ensemble methods represented by the lower edge (⇢ %), grouped by cheese variety. The number of observations can be found in Table 1 and colour codes in Fig. 4. Example for Emmentaler: *More than 90 mol% of the FVCAs originate from fermentations, which contribute approximately 70% to a correct classification (blue). Intensive fermentation, but weak proteolysis (red) are typical for Emmentaler.*

understand the impact of each feature on the classification of the cheese varieties, the SHAP value was calculated for the top three tree-based models. The interpretation of the SHAP value is a first step towards the differentiation of the cheese varieties. By comparing the relative amount of individual FVCAs with the relative SHAP value, a specific pattern can be recognised for each cheese variety (Fig. 5). Thus, it was possible to identify key FVCAs that could be applied as differentiating features as follows:

- Appenzeller®: the detection of C1 and of the iso-FVCAs;
- Berner Alpkäse: the detection of only low amounts of C3 and of the iso-FVCA;
- Berner Hobelkäse: the detection of C6 (and C4) and low proportions of C1;
- Emmentaler: the detection of high amounts of C2 and C3 and the absence of iso-FVCAs;
- L'Etivaz: the detection of C3 and iso-FVCAs;
- L'Etivaz à rebibes: the detection of C6 (and C4) and iso-FVCAs;
- Formaggio d'Alpe Ticinese: the detection of C1 and the absence of iso-FVCAs;
- Le Gruyère: the detection of C1, C3, and small amounts of iso-FVCA;
- Raclette du Valais: the detection of C1 and iso-FVCAs, as well as the absence of C6; and
- Sbrinz: the detection of low amounts of C1 and the absence of iso-FVCAs.

These unique feature combinations are always the result of specific characteristics of the cheese varieties: the detection of C1 is linked to the activity of citrate-metabolising lactic acid bacteria; the detection of iso-C4, iso-C5, and iso-C6 can be linked to the proteolytic activity of smear microbiota; and the detection of C6 is the result of lipolysis during ripening. Furthermore, C3 is a characteristic metabolite of propionic acid fermentation.

In conclusion, it was possible to classify 90% of the test data correctly by means of ML algorithms based on their FVCA profile. The application of the PyCaret library proved to be a simple, efficient, and promising tool for employment in research. The evaluation of the feature importance and especially of the calculated SHAP values proved to be highly informative. For similar ML applications, we recommend always evaluating the SHAP values, as they contributed substantially to the differentiation of the investigated cheese varieties.


## Funding

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.


## CRediT authorship contribution statement

**Marie-Therese Fröhlich-Wyder:** Conceptualization, Methodology, Software, Data curation, Writing – original draft, Visualization. **Hans-Peter Bachmann:** Conceptualization, Writing – review & editing. **Remo S. Schmidt:** Methodology, Supervision, Writing – review & editing.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

Data will be made available on request.

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