Free volatile carboxylic acids (FVCA) Every cheese has its own character

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In the first 20 years of this millenium, various compounds of 10 raw milk cheese varieties from Switzerland were analysed, including free volatile carboxylic acids (FVCA). These are among the analyses that are most frequently carried out, as they say a lot about the properties and quality of cheese.

As a logical consequence, the goal of characterising these varieties by means of FVCA was soon envisaged; however, a direct comparison was not made. This is now to be done by means of machine learning techniques, focusing on the following question: Can characteristic patterns be identified?



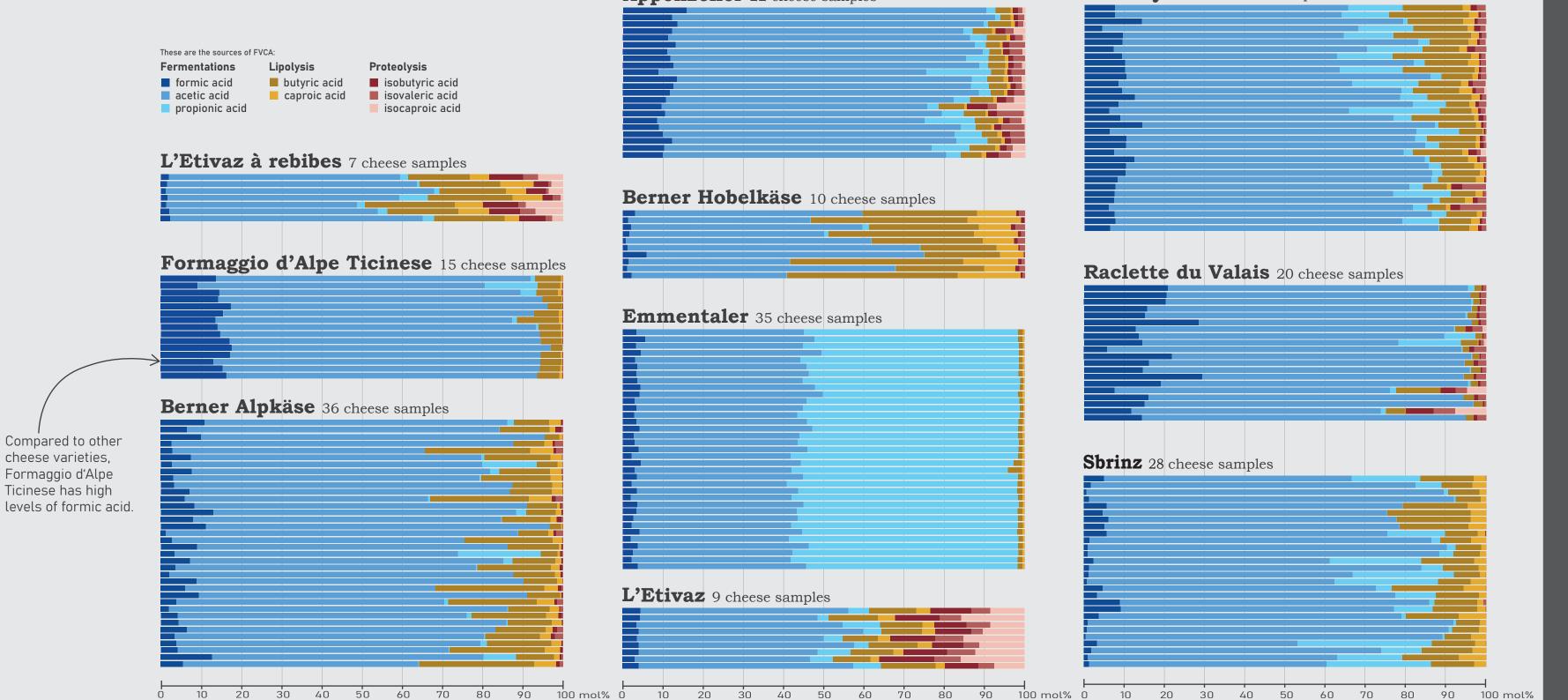
From the single values ...

The FVCA of 241 cheese samples of 10 different varieties were included in the investigation. Each horizontal bar represents one cheese sample.

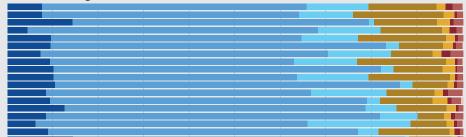
90% of the cheese samples can be correctly classified With the help of the PyCaret library, several algorithms could be tested in parallel. The best results were achieved with tree-based algorithms — Extra Trees and Random Forest. After the 10 training runs with 70% of the data, over 90% of the test data (the remaining 30%) could be correctly classified, a promising result.

isovaleric acid isocaproic acio

Appenzeller 22 cheese samples



Le Gruyère 33 cheese samples



Formic acid is the most important carboxylic acid

For a correct classification of the cheese samples, formic acid had the greatest impact. It is produced either by an added culture of facultative heterofermentative lactobacilli, as in Appenzeller® or Emmentaler AOP, or by the same bacteria originating from raw milk, as in Raclette du Valais AOP. In contrast, formic acid is less present in extra-hard cheeses, which in turn is characteristic of them. Carboxylic acids unimportant for classification were acetic acid and butyric acid.

Glossary

anaerobic metabolism of sugars and acids Fermentations : Lipolysis: hydrolysis of fat hydrolysis of proteins Proteolysis: SHAP: SHapley Additive exPlanations PyCaret: open-source, low-code machine learning library

... over the mean values

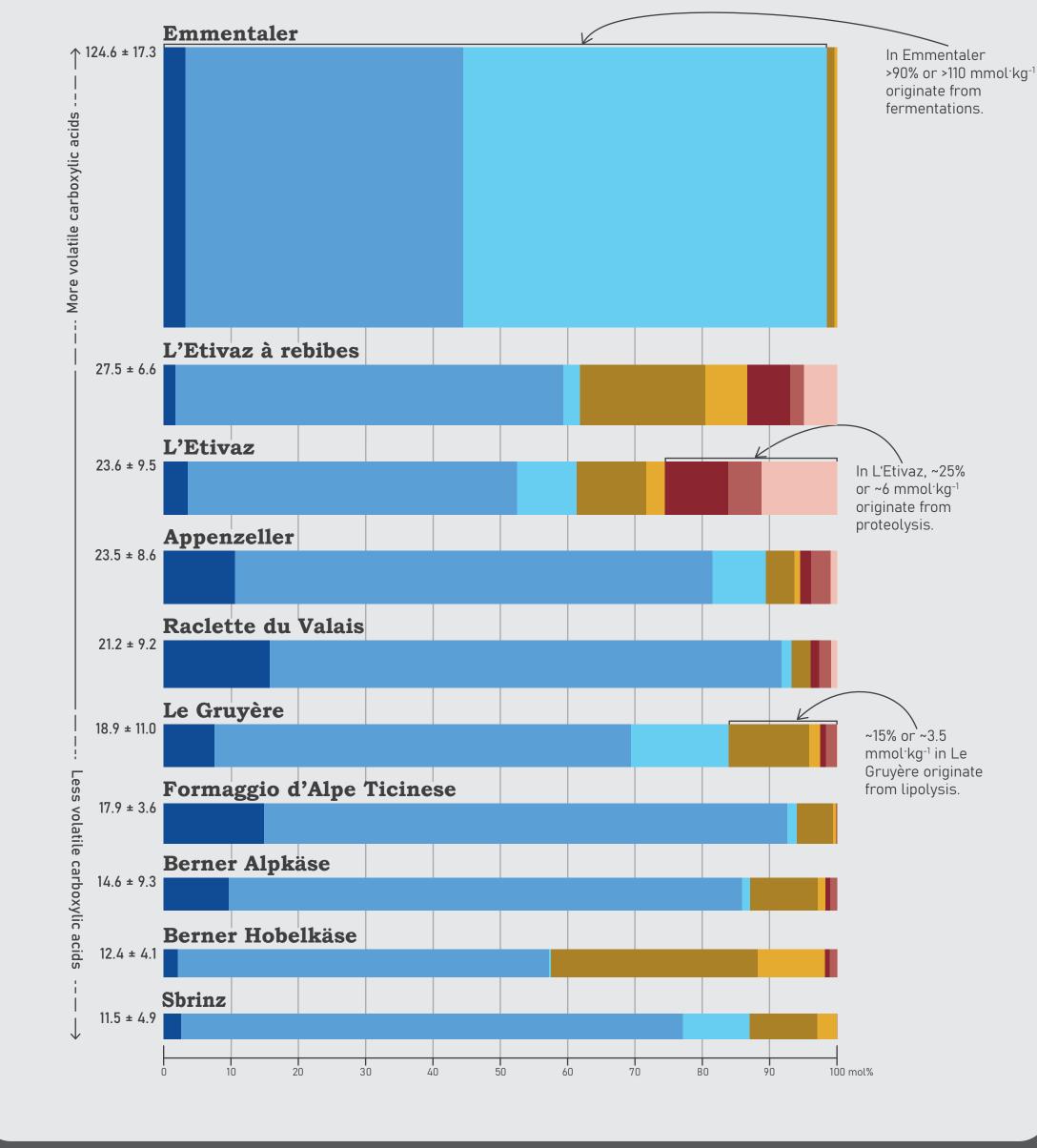
The mean values and standard deviations were calculated from the individual cheese samples for all varieties — which, with the exception of Appenzeller, carry an AOP label. The bar thickness represents the total amount of volatile carboxylic acids in 1 kg of cheese (mmol·kg⁻¹) and the length the proportions in mol%.

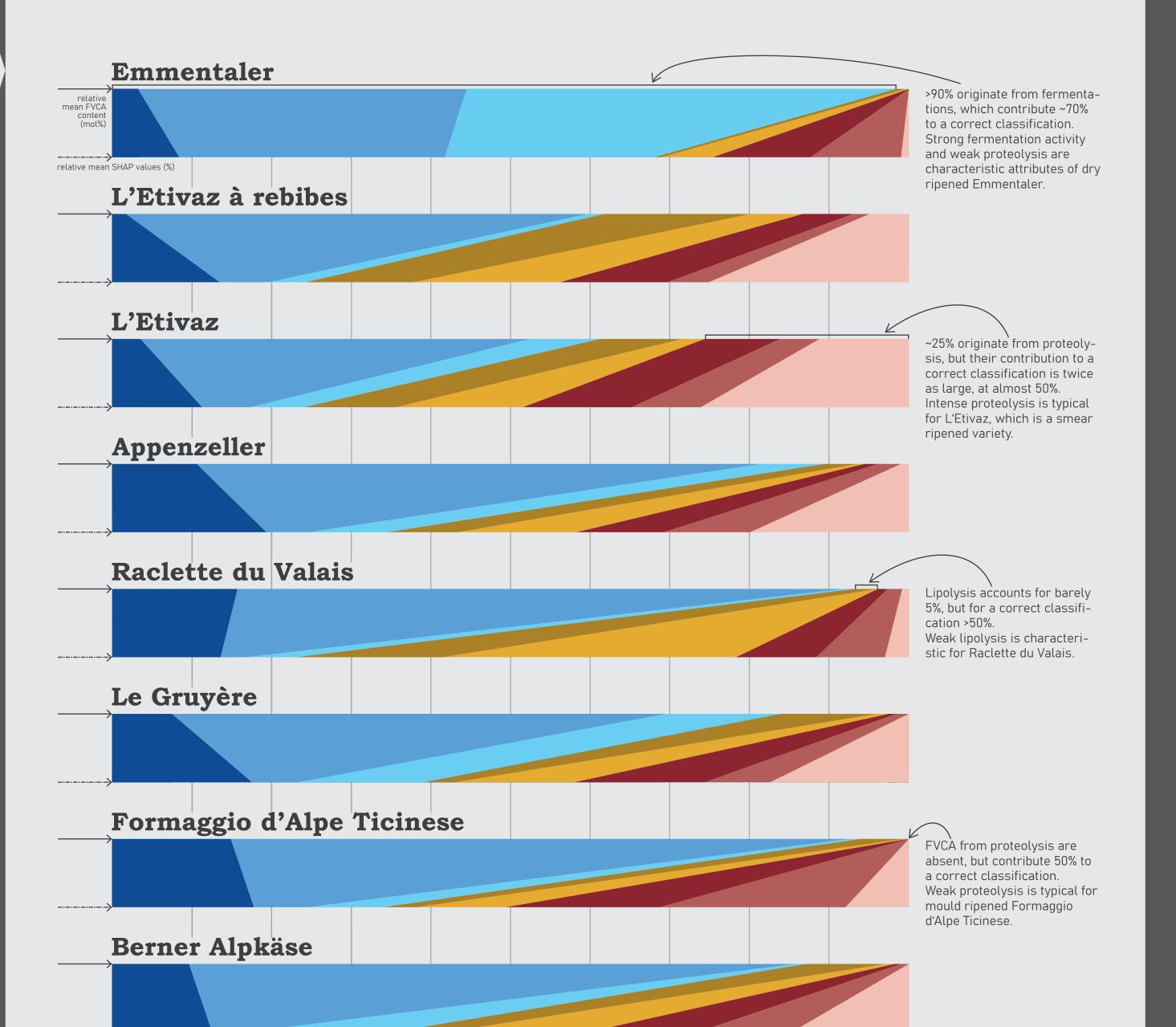
Emmentaler has the most FVCA at 124.6 ± 17.3 mmol·kg⁻¹ and Sbrinz the least at 11.5 \pm 4.9 mmol⁻ kg⁻¹. Regardless of whether a cheese variety has high or low levels of FVCA: the carboxylic acids from fermentations (blue) always predominate, especially acetic acid!

... to their significance.

Thanks to the SHAP values (SHapley Additive exPlanations), it was possible to define for each type of cheese those carboxylic acids that are important for its correct classification. They indicate how each carboxylic acid has

been weighted and thus reveal something about the typical character of a cheese variety. The combination of the FVCA with their SHAP values gives the cheeses a characteristic pattern.



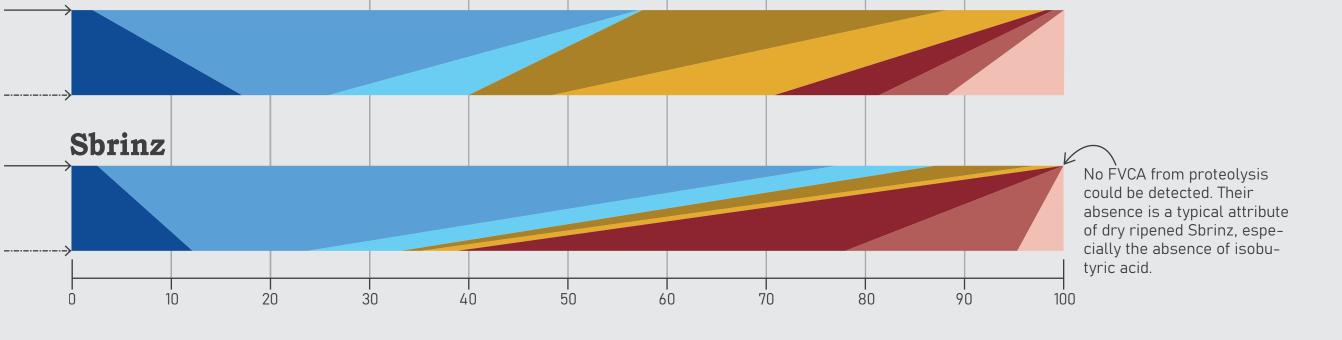


Conclusions

Based on the eight FVCAs, it was possible to classify 90% of the test data correctly by means of the machine learning algorithms Extra Trees and Random Forest. The most importat feature was C1, followed by C3, C6, and iso-C4. The application of the PyCaret library proved to be a simple, efficient, and promising tool; the evaluation of the feature importance and especially of the calculated SHAP values were highly informative.

The combination of the molar fraction of each FVCA with its importance, based on the SHAP values, led to a highly specific pattern for each cheese variety.

Berner Hobelkäse



Farmhouse and Artisan Cheese & Dairy Producers European Network

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