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Deeper Insight into Results of a Round Robin Test by Multivariate Data Analysis

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Introduction and Method

Between 2008 and 2016, under the guidance of VLB, 40 breweries took part in a round robin test to characterize 7 beer types from 6 different German breweries. Numerous independent scientists performed the standard tests by using similar methods and equipment. These data were measured as described in DIN ISO 5725 Part 1 and 2.
In many data structures there is a high redundancy of the measured parameters. Thus, a principal component analysis (PCA) is performed to extract the most important information. PCA is a chemometric method that splits a two-dimensional data table – in this case comprising 233 different samples and 11 different parameters – into a bilinear model of latent variables, the so-called principal components (PC). The principal components are calculated so that they explain as much variance of the data as possible. The objects, in our case the different beers, are then described in a lower dimensional PC space. A PCA allows a linearly independent clustering and structuring of the samples and facilitates the interpretation of the data.

Results and Discussion

The common way to describe the correlations between quality parameters is to calculate the correlation coefficients r. Table 1 shows the correlation coefficients for the 11 measured parameters. The intensity of the colour indicates the correlation strength. ‘Red’ means a positive correlation, ‘blue’ a negative one, ‘no colour’ indicates that there is no correlation.

	$E_{app.}$ W-%	$E_{re.}$ W-%	Alc. W-%	Alc. V-%	$E_{st.}$ W-%	pH-Value	CO_2	Bitterness	Colour	Foam	Turbidity
$E_{app.}$ W-%	1,00	0,97	0,75	0,74	0,85	0,68	0,35	-0,15	0,28	-0,08	-0,28
$E_{re.}$ W-%	0,97	1,00	0,88	0,88	0,95	0,76	0,17	-0,02	0,08	-0,05	-0,32
Alc. W-%	0,75	0,88	1,00	1,00	0,98	0,77	-0,22	0,22	-0,32	0,03	-0,41
Alc. V-%	0,74	0,88	1,00	1,00	0,98	0,78	-0,23	0,24	-0,33	0,04	-0,40
$E_{st.}$ W-%	0,85	0,95	0,98	0,98	1,00	0,79	-0,08	0,14	-0,18	0,01	-0,37
pH-Value	0,68	0,76	0,77	0,78	0,79	1,00	-0,01	0,29	-0,22	0,04	-0,26
CO_2	0,35	0,17	-0,22	-0,23	-0,08	-0,01	1,00	-0,58	0,53	-0,20	0,20
Bitterness	-0,15	-0,02	0,22	0,24	0,14	0,29	-0,58	1,00	-0,53	0,14	0,57
Colour	0,28	0,08	-0,32	-0,33	-0,18	-0,22	0,53	-0,53	1,00	-0,11	0,05
Foam	-0,08	-0,05	0,03	0,04	0,01	0,04	-0,20	0,14	-0,11	1,00	-0,03
Turbidity	-0,28	-0,32	-0,41	-0,40	-0,37	-0,26	0,20	0,57	0,05	-0,03	1,00
Legend	1,00	0,80	0,60	0,40	0,20	0,00	-0,20	-0,40	-0,60	-0,80	-1,00

Tab. 1: Correlation matrix of the different quality parameters

Extract (real and apparent), alcohol and the pH-value all show a correlation coefficient higher than 0.8. All the other parameters don’t show a clear correlation. This representation summarizes the measured parameters but does not classify the beers.
With a PCA it is possible to get a summary on how the correlations between the measured parameters are as well as a clustering according to the similarities of the beers. The beer clusters are shown in the scores plot (Fig. 1), and the correlations of the measured parameters are shown in the loadings plot (Fig. 2).

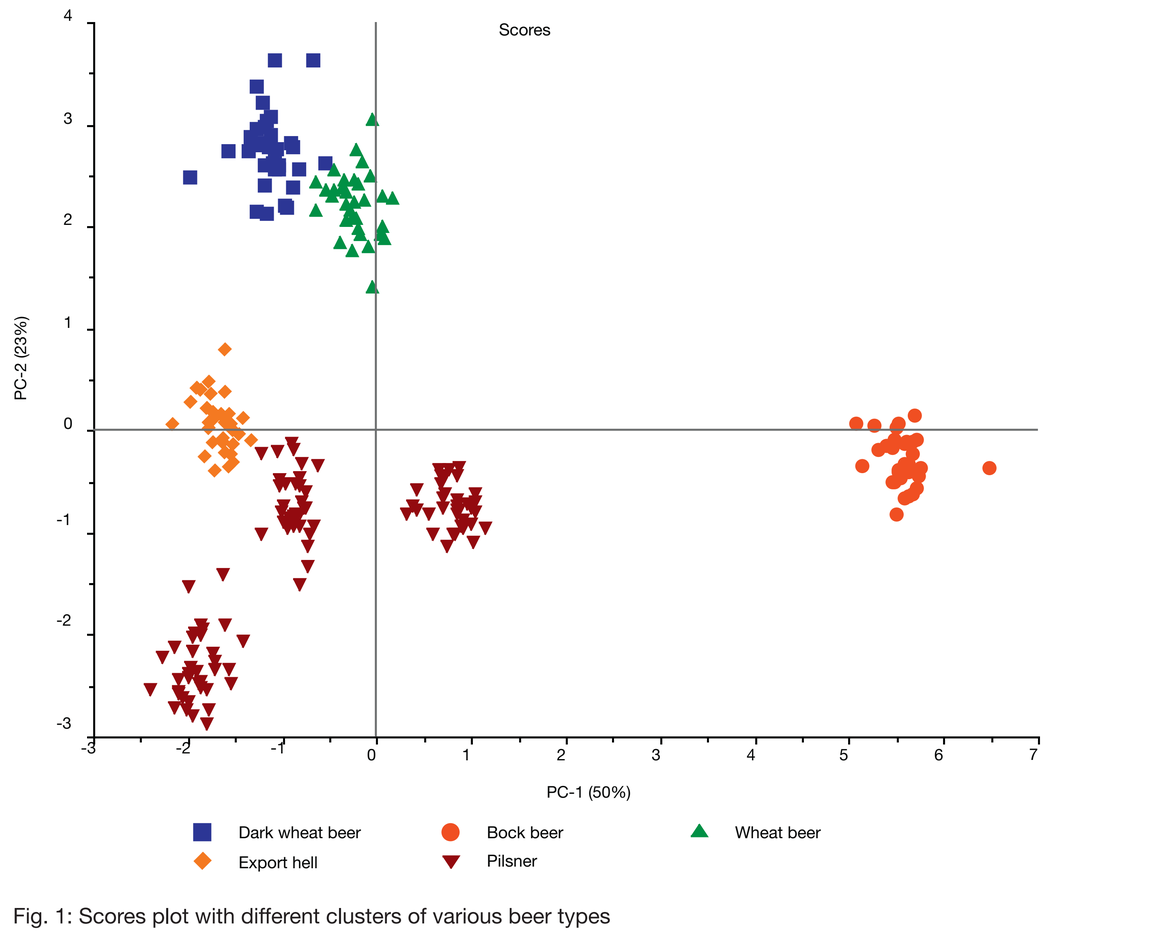

Fig. 1: Scores plot with different clusters of various beer types

The cluster of Bock beer is very different to the others. Bock beer has the highest score in PC 1 and Export hell the lowest. Surprisingly both are neutral to PC 2. The three different Pilsner beers can be differentiated mainly by PC 1 but also to a certain extend by PC 2. The results of the two different Wheat beers are very close to each other on PC 1 and PC 2.
Fig. 2 shows the loadings plot of PC 1 and 2. Alcohol (weight- and volume-%), extract (real and apparent) and pH-value represent PC 1 (see high correlations in table 1, mainly composition). PC 2 is orthogonal to PC 1 and represents mainly colour, CO_2 and also bitterness and turbidity which have different signs in the loadings (mainly appearance and taste). With regard to these data this means that beer with a higher CO_2 level has lower bitterness and turbidity on average. Neither PC 1 nor PC 2 inclose foam.

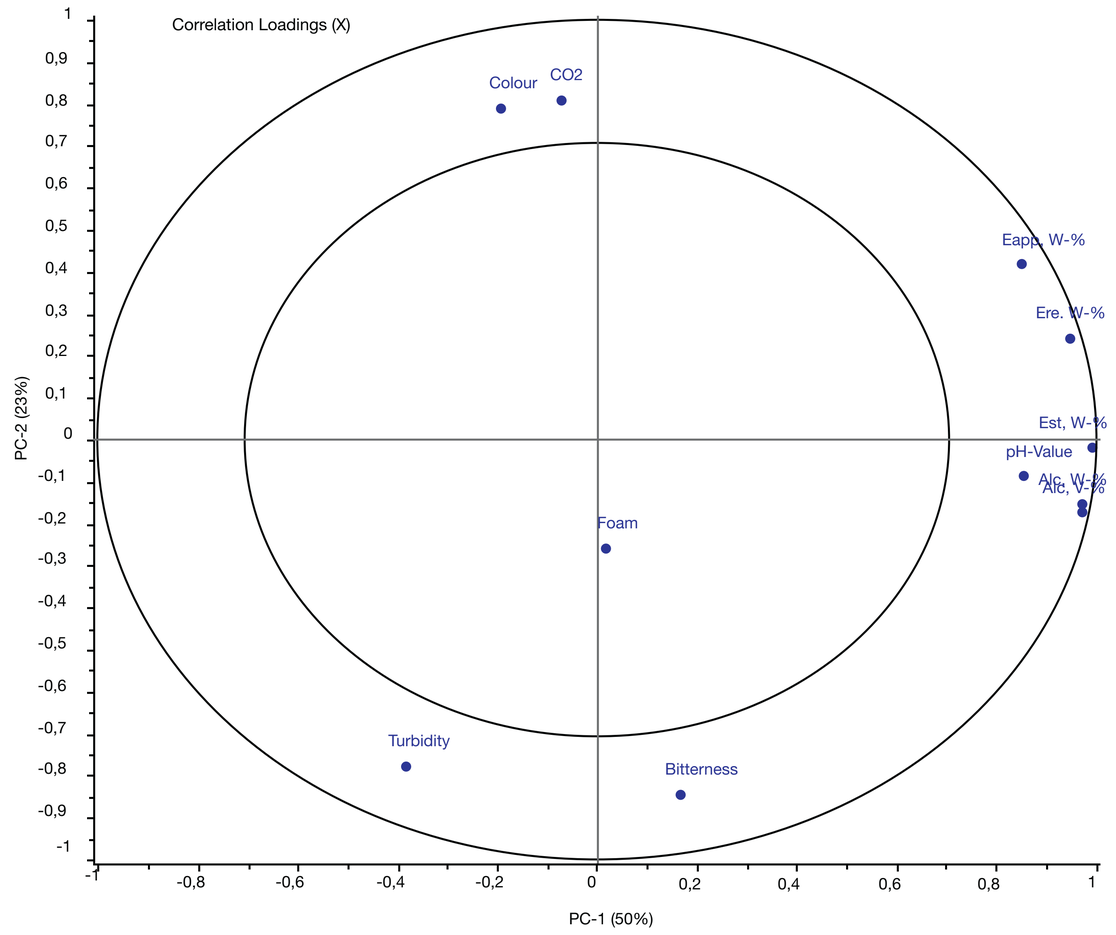

Fig.2: Loadings plot of the measured quality parameters

Conclusion and Perspectives

The PCA allows to characterize the measured quality parameters according to their intercorrelations. Despite the assumption that the same beer is produced all the time the PCA shows that the beers within one type (e.g. Pilsner) are different to each other. Approaches like the optical spectroscopy used as inline analysis could offer a chance to qualify the beers during production. This gives the opportunity for adapting the brewing process to a defined quality. These approaches have already been verified for different quality parameters in the beverage industry and will soon be expanded to more parameters.

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