How to Analyse Chemical Compounds? A Guide to Compositional Data Analysis Demonstrated with Beer Data

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In recent years, a lot of analysis was carried out to investigate data on chemical compositions of (non-)alcoholic beverages (whiskey, wine, beer, etc.) and food. However, no study has ever considered the compositional pitfalls inherent in such studies, which may lead to arbitrary results. Two approaches were compared, compositional data analysis (CoDa) and classical statistical analyses. The outcome of compositional data analysis methods provided very well-interpretable results. The method we are proposing is novel in the field of food chemistry, with demonstrated ability to analyse the chemical composition of drinks and food.

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1HOW TO ANALYSE CHEMICAL COMPOUNDS? A GUIDE TO
2COMPOSITIONAL DATA ANALYSIS DEMONSTRATED WITH BEER DATA

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4

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12

13Abstract

14In recent years, a lot of analysis was carried out to investigate data on chemical
15compositions of (non-)alcoholic beverages (whiskey, wine, beer, etc.). However, no
16study has ever considered the compositional pitfalls inherent in such studies, which
17may lead to arbitrary results. Two approaches were compared, compositional data
18analysis (CoDa) and classical statistical analyses, to demonstrate (i) how aging affects
19beer and (ii) how the results vary depending on the applied approach. Exemplarily,
20chemical compounds (aldehydes, ketones, esters) of 43 beer samples were analyzed.
21Our work has led us to obtain different results, when the analysis (correlation analysis
22and principal component analysis) was conducted on the unmodified-, log-
23transformed-, or closed-data in contrary to the analyses of log-ratio coordinates. The
24outcome of the latter provided very good separation between aged and fresh beer
25samples and well-interpretable results. The method we are proposing is novel in the
26field of food chemistry, with demonstrated ability to analyze the chemical
27composition of drinks (and food).

28

29Keywords

30chemical composition of drinks, chemometrics, log-ratio analysis, correlation, PCA

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32

331. Introduction

34 So far, hundreds of articles have been published about the chemical
35composition of beverages (eg. beer, coffee, wine, whisky, tea). Statistical techniques
36most often applied in such data treatment (Nunes et al., 2015) are cluster analysis,
37principal component analysis (PCA), response surface methodology, k-nearest
38neighbors and artificial neural networks. PCA is for instance widely applied to
39investigate samples of teas (Liu et al., 2014; Wu et al., 2015), tequilas and mezcals
40(another Mexican spirituous beverage; Muoz-Muoz et al., 2010), spirit drinks, wines
41and various beers (Varmuza et al., 2002; Mannina et al., 2003; Duarte et al., 2004;
42Almeida et al., 2006; Lachenmeier, 2007; Granato et al., 2011; Moura-Nunes et al.,
432016; Oladokun, 2016). Correlation analysis is also often used to characterize Indian
44beers (Pai et al., 2015), commercial lager beers (6 dark, 28 pale and 6 alcohol free;
45Blanco et al., 2015), also to show the antioxidant activities (Zhao et al., 2010) and
46phenolics content profile of various beer types (abbey, ale, bock, wheat, lager, pilsner,

47and dealcoholized; Piazzon et al., 2010). To understand the bitterness of dry-hopped
48beers, Parkin and Shellhammer (2017) used ANOVA and regression analysis, while
49for the characterization of flavour and the chemical composition of lager beers partial
50least squares regression was applied on the raw data by Saison (2010).

51 All these above listed studies have one in common: standard statistical
52methods were applied on compositions without considering the special nature of such
53data. When we look the reviews about the analytical and statistical methods used in
54food science and technology (Granato et al., 2014; Nunes et al., 2015), as well as in
55food chemistry (Kamiloglu, 2019), they do not mention compositional data analysis
56(CoDa; Aitchison, 1986). Food chemistry is a research field where plenty of
57compositional data are available, but where – up to our knowledge and intensive
58research – the scientific community does not use CoDa methods. If traditional
59statistical analysis is applied on compositional data sets, (i) correlations are well
60known to be arbitrary and even the (ii) arithmetic mean is not an adequate measure as
61the center of the distribution. This may lead to arbitrary results and potential wrong
62conclusions. Therefore, CoDa can be a way to gain additional insights and to see
63beyond a constrained space (simplex).

64 Compositional data are a quantitative description of the parts/compounds of
65some whole, conveying relative information (Aitchison, 1986; tbc in Section 1.4 and
662.2.1), which oft appear in food chemistry. Data can be compositional even if they are
67not closed; and there is no need to close them. It is a myth that compositional data
68sum up to 1 (or 100). Compositional data are typically being represented in
69proportions or percentages, but also in other units, like chemical elements in parts per
70million (ppm), mg/kg and mg/l, which reflect their relative nature. The relative
71information is the most important information about the smell and taste of drinks, the
72absolute numbers and the unit of measurement are less/non-informative. Another
73issue to consider are chemical processes, which may transform certain compounds
74into new compound(s) as described for ground water (Owen et al., 2016). If chemical
75compounds decrease (or increase) during a chemical process over time (the reaction
76between molecules), the decrease is measured on a relative scale and it is proportional
77to the whole. Some functional groups dissociate faster than others, but still the
78decrease is on a relative scale and not absolute (otherwise the concentration would get
79negative, which is practically impossible). In case of aging, the relative decrease to

the whole or other components is important, as it is demonstrated below with fresh and aged beers.

When an analysis is applied on compositional data that follows the “Principles of CoDa” (see, e.g., Mateu-Figueras et al., 2011; Boogaart and Tolosana-Delgado, 2013; Filmoser et al., 2018). (1) scale invariance: if a composition is multiplied by a constant the results won’t change; (2) permutation invariance: reordering of variables does not change the results; (3) subcompositional coherence is fulfilled if both holds (a) dominance: the distance between two compositions is greater equal the distance between a subset of the compositions; (b) ratio preserving: the information is included in the ratios and the information of non-selected variables does not influence the results if functions applied on subcompositions. As a result, analysis applied on the proportional/constrained data (each element of the vector is divided by its row sums) will give the same results as the analysis of the unconstrained data. The following simplified examples demonstrate the principles of CoDa. Changing the unit of one composition may automatically result in an outlier when standard outlier detection methods are applied (violating scale invariance), but results are unchanged if CoDa is applied. Consider two margarita cocktail (tequila, triple sec, orange juice); one is mixed by a Mexican barkeeper $x = (0.55, 0.40, 0.05)$ and the other is mixed by a French barkeeper who is fascinated from triple sec, thus $y = (0.10, 0.80, 0.10)$, expressed in proportional representation. Their Euclidean distance is $d(x, y) = \sqrt{[(0.55 - 0.10)^2 + (0.40 - 0.80)^2 + (0.05 - 0.10)^2]} = 0.604$. When only tequila and triple sec are measured, and the compositions expressed as proportions, i.e. $0.55/(0.55+0.40)$, etc., we get $x_s = (0.579, 0.421)$ and $y_s = (0.111, 0.889)$, their Euclidean distance is 0.661, which is higher than the distance of the whole compositions (violating subcompositional dominance). In addition, if an analysis (e.g. estimation of the correlation) is made on the subcompositions from samples containing the proportions of tequila and triple sec only, the results differ if the same analysis (e.g. correlation between tequila and triple sec) is made on proportions from all three components (violating ratio preserving). It can be also easily be seen that such a proportion cannot have larger values than 1, thus the correlation between compositional compounds is forced to be negative or at least to be low just as a result of the constrained space. One can show that Euclidean distances and standard statistical analysis are not suitable for compositions (see more examples

113in Filzmoser, Hron, Templ, 2018). However, to best of our knowledge, CoDa has
114some inherent drawback such as 'essential zeros', which does not allow to apply log-
115ratios in a straightforward manner. It is not easy, how to handle it, but first attempts
116have been made (Templ et al., 2017) - see further discussion on Section 2.2.1.

117 This study was motivated by our practical expertise and theoretical
118background on CoDa that chemists and data analysts in nutrient-, food- and hydro-
119chemical science may obtain additional insights into their data and receive better
120interpretable results when CoDa methods are applied. Compositional data analysis
121(CoDa) with classical statistical analyses were compared to demonstrate (i) the effect
122of aging on the chemical components of beer samples and (ii) how the results vary
123depending on the applied method (correlation analysis, principal component analysis).
124

1252. MATERIALS AND METHODS

126To demonstrate the application of CoDa methods in food chemistry, a dataset on
127chemical compounds of beers were used as an example. On a global level, beer
128consumption is much more important than wine or other alcoholic beverages in
129volume terms (Colen and Swinnen, 2011). Beer brewing is a process, which elaborate
130four essential raw materials, including barley malt, brewing water, hops and yeast.
131Particularly hops determine the typical beer qualities such as bitter taste, hoppy
132flavour, and foam stability (De Keukeleire, 2000; Schönberger and Kostecky, 2011).
133Beer experts can recognize a beer brand based on its constant, fresh flavor. However,
134beer-aging results in the production of stale flavors; thus, the original flavor is lost.
135This happens because the beer experiencing flavor deterioration, which is the result of
136both formation and degradation reactions during storage (Vanderhaegen et al., 2006).
137With, e.g., gas chromatography the chemical compounds of beers can be determined.
138It allows identifying the compounds of beer, which are responsible for the stale
139flavors.

140

1412.1. Beer samples

142In this study, 43 beer samples were re-analyzed from 14 breweries in Austria,
143Hungary and Romania provided by Varmuza et al. (2002). Their focus was to analyze
144the key volatile chemical compounds of beer samples, in particular the concentration
145levels of aldehydes, ketones and esters (for details see Table 1).

146

Table 1. List of analyzed chemical compounds (chemical name, abbreviation for figures, CAS Reg. No., chemical formula and taste characteristics obtained from PubChem and references therein, accessed 5.1.2019).

Chemical name	Abbreviation	PubChem CID	CAS Reg. No.	Molecular formula	Taste /or comments
3-methyl-butyraldehyde	3MeBu-al	11552	590–86–3	C ₅ H ₁₀ O	warm, herbaceous, slightly fruit and nut-like taste, apple-like odor
3-methyl-2-butanone	3MeBu-on	11251	563–80–4	C ₅ H ₁₀ O	flavoring agent
2-methyl-butyraldehyde	2MeBu-al	7284	96–17–3	C ₅ H ₁₀ O	almond, cocoa, fermented, hazelnut, malt
capronaldehyde	Hexanal	6184	66–25–1	C ₆ H ₁₀ O	characteristic fruity taste and green, woody, vegetative, apple, grassy, citrus and orange with a fresh lingering aftertaste
2-(hydroxymethyl)-furan	2FurMeol	7361	98–00–0	C ₅ H ₆ O ₂	burnt, caramel, cooked
heptaldehyde	Heptanal	8130	111–71–7	C ₇ H ₁₄ O	citrus, fat, green, nut
2-furyl methyl ketone	2AcFur	14505	1192–62–7	C ₆ H ₆ O ₂	flavoring agent
5-methyl furfural	5Me2Fur	12097	620–02–0	C ₆ H ₆ O ₂	flavoring agent
furfuryl acetate	EssFuEst	12170	623–17–6	C ₆ H ₆ O ₃	fruit
2-acetyl-5-methyl furan	2Ac5MeFu	14514	1193–79–9	C ₇ H ₈ O ₂	nutty-like flavoring
benzene acetaldehyde	2PhEt-al	998	122–78–1	C ₈ H ₈ O	honey-like, sweet, rose, green, grassy smell
nicotinic acid ethylester	NicEtEst	69188	614–18–6	C ₈ H ₉ NO ₂	flavoring agent
ethyl phenylacetate	2PhEssEt	7590	101–97–3	C ₁₀ H ₁₂ O ₂	tasting sweet and fruity
gamma-nonanoic lactone	gNonalac	7710	104–61–0	C ₉ H ₁₆ O ₂	coconut, creamy, waxy with fatty milky notes
furfural	Furfural	7362	98–01–1	C ₅ H ₄ O ₂	flavor ingredient. Beer decreases in taste with higher

					concentrations of furfural. Toxic oil with a bitter smell
5-hydroxymethyl-2-furancarboxaldehyde	HMF	237332	67–47–0	C ₆ H ₆ O ₃	flavoring agent

150

151

152 Observations were made on fresh beer samples (they were stored at 10°C for 14
153 days), as well as on the same beers after artificial aging. The beers were aged by
154 constantly storing them at 45°C for 2 weeks. The chemical measurements of
155 compounds were detected before and after the aging by using gas chromatography–
156 mass spectrometry (GC/MS; Sparkman et al., 2011), after steam distillation (Glinser,
157 1999). Only one substance, 5-hydroxymethyl-2-furancarboxaldehyde was analyzed by
158 HPLC (Leubolt and Klein, 1989). The units of the measurements/concentrations are
159 expressed in µg/l. It is obvious that not the absolute values determine the flavor of the
160 beer, but the ratios of variables are important.

161

162 2.2. Data analysis

163 2.2.1. Log-ratio analysis of compositional data

164 The sample space of the beer compositional data was defined (after Filzmoser et al.,
165 2018) as follows:

$$166 \quad S^D = \{x = (x_1, \dots, x_D)' \in R_+^D \mid \forall \kappa > 0 \exists \lambda > 0 : x = \lambda C_\kappa(x)\}$$

167

168 The aim of log-ratio analysis is first to find an orthogonal representation (=log-ratio
169 coordinates) of the compositional data in the Euclidean space. The compositions can
170 be mapped from S^D to the real space R^{D-1} by using the family of (isometric) log-
171 ratio transformations. One possible representation of compositional data in R^{D-1}
172 are pivot (log-ratio) coordinates (Filzmoser et al., 2018). They are based on the
173 isometric log-ratio coordinate representation (Egozcue et al., 2003) and they form an
174 orthogonal basis, given by

$$175 \quad \text{ilr}(x) = z = (z_1, \dots, z_{D-1})' \quad \text{with} \quad z_j = \sqrt{\frac{D-j}{D-j+1}} \log \frac{x_j}{\sqrt[D-j]{\prod_{k=j+1}^D x_k}} \quad \text{for}$$

$$176 \quad j = i, \dots, D-1.$$

177

178 As it can be seen, the first variable x_1 only appears in coordinate z_1 , while
 179 x_2 , for example, appears in both z_1 and z_2 . z_1 can thus be interpreted as
 180 the relative dominance of x_1 with respect to the other variables on the average.
 181 The interpretation of results is mostly done using the coordinate representation. Thus,
 182 when interpreting the results of a CoDa analysis, the interpretation should rely on the
 183 log-ratio coordinates and not on the original representation of the data in S^D .

184 It must be mentioned that CoDa has an inherent drawback, namely the
 185 problem related to “essential zeros”; the log-ratios are not defined, because of having
 186 a zero in the numerator or denominator of the ratio. There have been several zero
 187 replacement strategies suggested by Martín-Fernández et al. (2003), Martín-
 188 Fernández and Thio-Henestrosa (2006) and by further authors who have tried to
 189 contribute to solve this problem (Fry, McLaren, Fry, 2000; Aitchison and Kay, 2003;
 190 Bacon-Shone, 2003; Wang et al., 2007; Butler and Glasbey, 2008; Scealy and Welsh,
 191 2011; Martín-Fernández et al., 2015; Templ, Hron, Filzmoser, 2017; Tsagris, Steward,
 192 Lobachevskii, 2018; Chong and Spencer, 2018). Most of these approaches were
 193 reviewed by Filzmoser et al. (2018).

194 Depending on the desired application, other representations in (orthonormal)
 195 log-ratios might be preferable. Often, specific subsets of parts are of interest in
 196 contrast to another subset of parts, which helps in the interpretation of the results. In
 197 such cases, other log-ratios are defined via so called balances instead of the pivot
 198 coordinates (for details, see Filzmoser et al., 2018 or Egozcue and Pawłowski-Glahn,
 199 2005).

200 In this study, the composition of the beer samples using log-ratio analysis on
 201 centered log-ratio (orthogonal) coordinates were evaluated. The coordinates were
 202 obtained by applying a centered log-ratio transformation (Aitchison, 1986), namely by
 203 dividing each value of a composition of the geometric mean of the composition and
 204 then taking the logarithm. Besides pairwise log-ratios, centered log-ratio coordinates
 205 are often used in compositional biplots, because of their simplicity and symmetry

206(Aitchison and Greenacre, 2001; Filzmoser et al., 2009).

207

208**2.2.2. Correlation analysis**

209Measuring the linear dependency between (two) variables is a frequently applied
210method for the analysis of chemical compounds. As already outlined by Pearson
211(1896), computing the correlation between two variables is inappropriate whenever
212the sample space of data is a simplex. It happens because the value automatically be
213forced towards a lower positive or a higher negative one.

214 Variation is one specific CoDa counterpart of a classical correlation (Aitchison
2151986). Here, the variance of log-ratios instead of classical correlation measures were
216calculated. Thus, the variation of Furfural and Hexanal is for instance defined as the
217variance of $\log(\text{Furfural} / \text{Hexanal})$. If the variation is low, the “correlation” is high.
218If the variation is high, the “correlation” can be said to be low, i.e. the ratios of these
219two variables differs a lot. Namely, the lower the variation, the stronger the
220correlation. Furthermore, perfect dependency of two parts is given, whenever the
221variation is zero. The Pearson correlations coefficients with their variations were
222compared to indicate the differences on the results and interpretation.

223

224**2.2.3. Principal component analysis (PCA)**

225PCA allows new projections of the original data to be obtained. Namely, the first
226principal component (the first score vector) is the linear combination of the variables
227of a data set for that it's projected values has the largest variance, thus explaining
228most of the data. PCA is frequently applied to concentrations of drinks and typically
229used for dimension reduction purposes or as an exploratory method to interpret the
230multivariate dependencies in the data set. For the latter one, the resulting first two
231(orthogonal) PCAs are often visualized in a biplot. A biplot allows you to visualize the
232magnitude and sign of each variable's contribution to the first two or three principal
233components, and how each observation is represented in terms of those components.

234 Various biplots were compared resulting from PCAs applied on (1)
235unmodified compositional data, (2) scaled and centered log-transformed
236compositional data, (3) closed data (the values are divided by the row sum), and on
237(4) log-ratio coordinates (the correct approach). The approach (4) means that the
238compositions are represented by (log-ratio) coordinates in the real (Euclidean) space
239by first applying a centered log-ratio transformation (Filzmoser et al., 2009). For (1-3)

240the correlation matrix (instead of the covariance matrix) was used as input to PCA,
241thus the scaled version of PCA.

242Note, that the effect of CoDa on the outcome is independent from the scale (or change
243of the scale) of the units of the chemical compounds.

244 All analyses were performed using the software and environment R (R
245Development Core Team 2016) and the R package “*robCompositions*” (Filzmoser et
246al., 2018).

247

2483. Results and Discussion

2493.1. Comparing results of the correlation analysis

250The correlation and variation between the chemical compounds of fresh and aged
251beers are shown on Fig 1. The classical correlation analysis of the compounds of
252beers (first column of Fig. 1) does not show much difference between fresh beers
253(first row of Fig. 1), aged beers (second row of Fig. 1), and between all beers analyzed
254together (last row of Fig. 1). The reason is that the correlation is already determined
255by the compositional nature of the data. In this case, large values of an unconstrained
256compositional data set drive the classical correlation positive and make the classical
257correlation results arbitrary (see 2.2.2).

258 A different picture can be drawn for the variation of fresh beers (Fig. 1, top
259right) as it is compared with the correlation matrix of fresh beers (Fig. 1, top left). For
260the aged beers (second row of Fig. 1) such differences are more pronounced. A low
261“correlation” (high variation) can be recognized between two substances
262(2AC5MeFu, EssFuEst) compared to all other compounds, however the variation of
263the other compounds does not differ to a great extent (middle right graphics of Fig. 1).

264

265
 266**Fig. 1.** Correlation (graphics on the left side) and variation (graphics on the right
 267side) between the compounds of beers. The first row shows the results from fresh
 268beers, the second row those from the aged beers, and the last row shows the results
 269for all beers together (fresh and aged).

270
 271The variation matrix of the fresh and aged beers (lower right graphic of Fig. 1.)
 272highlights, that the overall variation is driven by Furfural (a toxic oil characterized by
 273a bitter smell), which is known to increase in aged beers (Brenner and Khan, 1976). In
 274contrary, almost no changes in the compounds of aged beers can be observed based on
 275the classical correlation matrices (left graphics of Fig. 1.).

276 2773.2. Comparing results of various PCAs

299 still rather low (45,2%). This is basically equivalent to the results of Varmuza et al.
 300 (2002), which provided the motivation for further investigation of the dataset.

301

302 **Fig 3.** Biplot resulting from PCA applied on log-transformed compositional data. For
 303 abbreviations see Fig. 2.

304

305 When the compositional values are closed to 1 (or 100), it is difficult to interpret the
 306 resulting biplot (Fig. 4), especially because the various compounds are located in a
 307 half-space. It can be concluded that all solution (Fig. 2, 3, 4) are spoiled and arbitrary
 308 by disrespecting the nature of the compositional data. In addition, the explained
 309 variance of the first two principal components is very low.

316

317 **Fig. 5.** Biplot resulting from PCA on log-ratio coordinates. For abbreviations see Fig.
3182.

319

320 Since the latter biplot (Fig. 5) is in compliance with the principles of CoDa, the
321 arrows (indicating the compounds of the beers) are no longer distorted in a half-space
322 and the cosine's of the angle between the arrows approximates the correlation
323 between the log-ratio coordinates. Furthermore, a very good separation between aged
324 and fresh beer samples are observable; thus, the interpretation is much easier than in
325 any other previously discussed biplots (Fig. 2, 3, and 4).

326 Furfural has the strongest impact on the first principal component (PC; Fig.
327 5.), explaining the variance in the dataset. The aged beers pointing towards this
328 direction, indicating that the content of Furfural increased (a lot) in the samples of
329 aged beers. It can be observed that heptaldehyde (Heptanal) and 5-hydroxymethyl-2-
330 furancarboxaldehyde (HMF) are highly correlated with Furfural and associated with
331 the compounds of aged beers. While fresh beers have fruitier, more cocoa, almond
332 and caramel taste, since the 2MeBu-al, 2 FurMeol and EssFuEst compounds appear
333 on the biplot in positive direction with the first PC. It is to be noted that the group of
334 samples in the upper part are samples from a single brewery (not shown in Fig. 5).
335 These samples were determined by 2Ac5MeFu (organoleptic with nutty-like

336flavouring), benzene acetaldehyde (2PhEt-al, with honey-like, sweet, rose, green,
337grassy smell), ethyl phenylacetate (2PhEssEt, tasting sweet and fruity), 2-furyl methyl
338ketone (2AcFur, a flavoring agent) and 3-methyl-butylaldehyde (3MeBu-al, slightly
339fruity and nut-like, herbaceous). Not only Furfural, but other compounds increased
340with aging in samples of this brewery, e.g. 2PhEt-al and 2PhEssEt.

341 The main difference recognizable on Fig. 5., compare to the previous Figures,
342is that the explained variances of the first two principal components increased to
34356.4%. Note that Varmuza et al. (2002) had difficulties explaining the biplot
344originated from classical PCA applied on log-transformed compositions of the same
345beer dataset. They found (Varmuza et al. 2002) for instance that a special strong fresh
346beer and some Romanian fresh beers had the same flavor (chemical composition) as
347some aged beers. Such questionable pattern cannot be observed using CoDa approach.
348It should be mentioned that other, more sophisticated isometric log-ratio coordinates
349may give further insights about the compounds of beers. For instance, such coordinate
350could be investigated, which consist the log-ratio of the geometric mean of the
351compounds that indicate fruity tasting against the geometric mean of herbaceous
352compounds.

353

3544. Conclusions

355Compositional data analysis (CoDa) has been proposed for the investigation of
356chemical composition of beverages demonstrated using beer data. This study has
357highlighted that correlation analysis conducted on raw (unmodified) compositional
358data is problematic, because it becomes spoiled. The research also revealed huge
359differences between the results of the PCAs, when the analysis was conducted on the
360unmodified-, log-transformed-, or closed-data in contrary to the log-ratio coordinates.
361The later one leads to better interpretation, higher explained variance and is
362theoretical sound. The beer data only served as one example data set from food
363chemistry. However, the method we are proposing is novel in the field of food
364chemistry, with demonstrated ability to analyze the chemical composition of drinks
365and food.

366

367Taken together, these findings suggest to (1) check your data if it is compositional,
368and if it has a compositional nature, (2) use CoDa methods to analyze it.

369

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372 beer datasets and for his open mind to rethink the approach of analyzing this data set.
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380

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