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Comparability problems in the analysis of multiway data ☆

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ABSTRACT

Almost all methods for the analysis of multiway data assume that the comparison of any two entries in the data array under study reflects or represents meaningful content-specific information. This is especially the case if one wants the data analysis to yield insight into the real mechanisms underlying the data. Violation of this assumption may imply data-analytic results that are of doubtful quality at best and worthless in the worst-case scenario. In the present paper, we first clarify why comparability is a key assumption in most methods for multiway data analysis. Next, we list a number of reasons why this assumption is very often violated in practice. We then review a few possible approaches that have been advanced to deal with problems of comparability, and discuss their advantages and shortcomings. We conclude by clarifying that any satisfactory solution to comparability problems requires a very careful reflection about the data collection and the ultimate goal of the data analysis.

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1. Introduction

Assume a three-way sample by metabolite by timepoint data array with entries d_{ijk} pertaining to the (relative) intensity in sample i of metabolite j at timepoint k. Assume further that the scientific question the metabolomics researcher wants to address pertains to unveiling the biological mechanisms underlying those data.

To deal with this question, the researcher may use the following (PARAFAC) model:

$$d_{ijk} = \sum_{p=1}^{P} a_{ip} b_{jp} c_{kp} + e_{ijk} = \hat{d}_{ijk} + e_{ijk}. \quad (1)$$

In view of the ultimate goal of unveiling biological mechanisms by means of this model, one may wish the parameters of the model (i.e., the elements of the component loading matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$) to represent biologically relevant, structural characteristics respectively of samples, metabolites, and timepoints. Similarly, one may wish the entire model Eq. (1) to represent a biologically meaningful mechanism.

Assuming that this is the case, we may return for a moment to the data. Suppose that Fig. 1 contains the data slice pertaining to Timepoint 1. We then may wonder to which extent the numbers in this figure can be meaningfully compared, in the sense that comparisons of numerical values do reflect or represent meaningful biological information. Note that comparisons of numerical values are to be understood here in the sense of at least rank order (and optionally on top of that also in the sense of the magnitude of differences or ratios). Hence, we face the question whether the rank order of any two numbers in Fig. 1 is meaningful from a biological point of view.

Now, it looks fairly obvious that different values in the same column (e.g., 10, 12, 8, 10 and 6) can be compared directly: They reflect different intensity values of the same metabolite in the different samples and have a meaning in terms of underlying concentrations. However, comparisons across columns (in the rows) are problematic. For example, what is the biological meaning of the difference between 10 and 12 in the first row? Does this difference imply the same interpretation as the difference between 10 and 12 in the first column? A critical underlying problem here is of course the difference in instrumental response factors (i.e., the translations from instrumental responses to concentrations) for the metabolites. Otherwise, even after proper calibration, the problems are not yet solved, as will be shown later in this paper.

Unfortunately, a lack of full comparability of the data entries implies a major problem for the intended data analysis. There are at least two major reasons for this:

(1) For the parameters of the PARAFAC model (i.e., the elements of the component loading matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$) to represent

☆ This paper is dedicated to the memory of Richard Harshman.

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	metabolites		
samples	1	2	3
1	10	15	12
2	12	10	8
3	8	5	4
4	10	..	..
5	6	..	..

Fig. 1. Sample by metabolite intensity data at timepoint 1.

biologically relevant, structural characteristics of samples, metabolites, and timepoints, and for the PARAFAC model equation to represent a biologically meaningful mechanism, comparability of the (reconstructed) data entries is of key importance. To clarify this, let us revisit the lack of a biological interpretation of the difference between 10 and 12 in the first row of Fig. 1. The reconstructed data entries corresponding to these two numbers are $\hat{d}_{111}$ and $\hat{d}_{131}$. Now, according to the PARAFAC model, the difference between these two numbers is to be entirely attributed to the difference between the component loadings of the first and third metabolite, (b_{1p}, $p=1,\ldots,P$) and ($b_{3p}, p=1,\ldots,P$). Yet, if the difference between $\hat{d}_{111}$ and $\hat{d}_{131}$ cannot be given a sound biological interpretation, the hope for the metabolite loadings as contained in $\mathbf{B}$ to represent biologically relevant, structural characteristics of the metabolites cannot be but vain.

(2) The estimation of the PARAFAC model is typically based on the minimization of the following loss function:

$$\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}\left(d_{ijk}-\hat{d}_{ijk}\right)^2=\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}e_{ijk}^2. \quad (2)$$

This loss function includes an addition over the full data array. For such an addition to be meaningful, one needs to presuppose that all residuals, and, hence, all (reconstructed) data entries are expressed on the same measurement scale. This assumption can be denoted by the term *commensurability*. In the vernacular, addition in absence of such commensurability is called 'addition of apples and oranges'. Obviously, in the metabolomics example, the failure to arrive at meaningful interpretations of within-row comparisons in data slices, like the one represented in Fig. 1, casts a serious doubt about the commensurability assumption.

Lack of comparability of data entries is a major problem in the analysis of multiway data. If not dealt with properly, the results of the analysis are of doubtful quality at best and worthless in the worst-case scenario. Amazingly, however, this problem is very often ignored in practice. Otherwise, one might perhaps expect that comparability problems can be rectified quite easily (e.g., in the metabolomics case, by making use of suitable calibration information). However, as we will explain below, the situation is far less easy as one may hope.

The structure of the remainder of this paper is as follows: we will start by clarifying how comparability of data entries is often implicitly required in most approaches to multiway data analysis (Section 2). Subsequently, we will discuss a series of major obstacles to comparability (Section 3). We then will move on to a review of a number of solutions that have been proposed so far to deal with comparability problems (Section 4), along with a discussion of their strengths and shortcomings (Section 5). We will end with a few concluding remarks in Section 6.

2. Requirement of comparability in most approaches to multiway data analysis

In a typical analysis of multiway data, comparability of the data entries is almost always assumed, although very often only implicitly. There are two possible reasons for this assumption. A first one is to be situated at the level of the actual multiway models, and a second one at the level of the data analysis. We will now successively discuss each of those two.

2.1. Conceptual model

Comparability becomes critical at the level of the multiway model whenever the goal of the data analysis goes beyond a mere data reduction or a purely exploratory analysis. This means that one really cares about the *conceptual model* of the system that generated the data [1]. Ultimately, this conceptual model should provide a ground for a content-specific interpretation of the estimated data-analytic model.

For a better understanding of this, one may refer to Fig. 2. Measurements taken from a biological system only probe certain parts of that system (red and green parts). Using a priori biological knowledge, a conceptual model of the system is made, especially of the parts that have been measured (this is sometimes called the data-generating process). The conceptual model is then implemented into a mathematical/data-analytic model, which is subsequently fitted to the data. For the mathematical/data-analytic model to be really useful, the parameters of this model as well as the actual model equation(s) should be interpretable in terms of the conceptual model. This implies that the parameters in question should have a clear and unambiguous biological meaning. Otherwise, one may note that interpretation is meant here in a broad sense: it also includes all kinds of model diagnostics and validation statistics.

As an example, we may revisit the PARAFAC model of Eq. (1). From an inspection of the model equation in question, it should be clear that, if this model would provide an isomorphic representation of the data-generating process, then this process necessarily depends on invariant and quantifiable structural characteristics of the elements of the different data modes as represented by the loading matrices. Note at this point that the term *structural* refers to in-built features of the

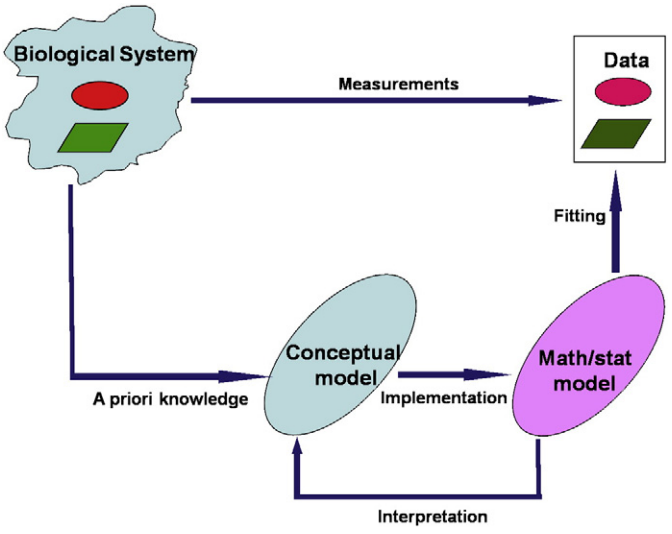


Fig. 2. Schematic representation of relations between biological system, data, conceptual model, and mathematical/data-analytic model.

elements of the data modes, and *invariant* to the fact that the relevant characteristics of an element of a data mode, as quantified by the corresponding row in its loading matrix, are the same irrespective of the combination of elements of the other modes under study.

To further clarify the above, we may consider a physicochemical context in which a PARAFAC model may be an adequate implementation of an underlying conceptual model, namely in the case of fluorescence spectral data (sample by excitation wavelength by emission wavelength). Fluorescence refers to light emission by certain molecules (fluorophores) when excited by photons. We then may consider the fluorescence intensity of a sample containing a single type of fluorophore p at a certain emission wavelength when being excited at a certain excitation wavelength. On the basis of physicochemical principles, this fluorescence intensity can be assumed to be proportional to the product of: (a) the molar concentration of the fluorophore, (b) the extent to which the fluorophore absorbs at the excitation wavelength (molar absorptivity), and (c) the efficiency of the fluorescence process for the fluorophore in question (quantum yield), which depends on the emission wavelength. For samples containing multiple kinds of fluorophores $p=1,\ldots,P$, in a number of cases (such as dilute solutions), the different kinds of fluorophores can be assumed not to interact. This finally yields an addition of multiplicative terms that can be implemented into a PARAFAC model [2]. In such a context, indeed, the PARAFAC model Eq. (1) and the PARAFAC parameters can be given a clear physicochemical interpretation, with the loadings of the samples representing relative concentrations, and with the other two loading matrices representing pure excitation and emission spectra.

The essential implication of all this now reads as follows: if the parameters and model equations of a mathematical/data-analytic model under study have to be meaningful from the point of view of an underlying conceptual model, then the same should also hold for the (reconstructed) data entries. This means that the numerical values of those entries should have a content-specific (e.g., biological) meaning. As a further consequence, the relations between those numerical values (e.g., rank order) should also be meaningful, which implies comparability of the entries in question.

As an aside, one may note that the above only works well in case of a very close (and preferably one-to-one) relationship between the conceptual and mathematical/data-analytic model. This further implies that the conceptual status of models that are not identified is necessarily less clear. As an example in this context, one may think of multiway models that are cursed with identifiability problems because of rotational freedom (such as the Tucker family of models).

2.2. Loss function

Many deterministic methods for multiway data analysis will optimize a least squares loss function such as (2), which implies an addition over the full data array. As already indicated in the Introduction to this paper, for such an addition to be meaningful, one needs to presuppose that all (reconstructed) data entries are commensurable. Otherwise, provided suitable independence assumptions on the residuals, the log likelihood function that is maximized in the estimation of stochastic multiway models includes an addition over the full data array similar as the one in (2).

3. Obstacles to comparability

In this section we will review two major obstacles to comparability. Both of them occur very often in data-analytic practice.

3.1. Conditionality

In the psychometric and mathematical psychological literature, already many years ago it has been pointed out that measurement characteristics of data entries may be conditional on aspects of the procedure through which the data have been collected, in the sense that some data entries cannot be meaningfully compared with other data entries [3]. Given data that have been organized in a two-way matrix, the case in which all data entries can be meaningfully compared is denoted by matrix-conditionality. If meaningful comparisons can only be made within one and the same row, this is denoted by row-conditionality, whereas the case in which meaningful comparisons can only be made within one and the same column is denoted by column-conditionality. Similarly, we may consider the three-way case, making use of the terminology as proposed in [4] and as graphically represented in Fig. 3. One may now draw a distinction between array-conditionality, (horizontal, lateral, and frontal) slice-conditionality, and (horizontal, vertical, and depth) fiber-conditionality. To clarify the concept of conditionality, we will illustrate this by means of three examples.

As a first example, we consider a two-way data set pertaining to a set of patients (rows) that have been measured on a set of clinical marker

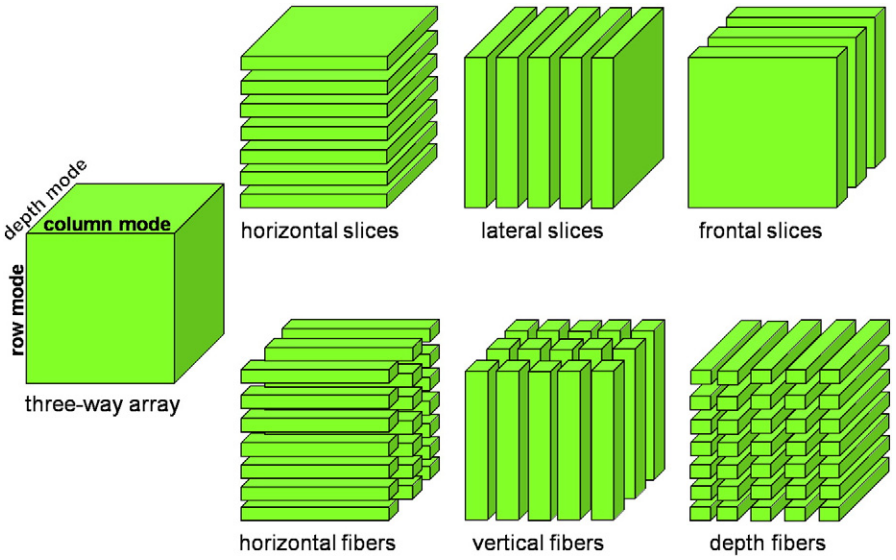


Fig. 3. Subdivision of three-way array in horizontal, lateral, and frontal slices, and in horizontal, vertical, and depth fibers.

variables (columns). The markers in question include blood pressure, body temperature, and the blood concentration of some antigen. Because different clinical markers are expressed in different measurement units, this is an obvious example of column-conditional data.

As a second example, we revisit the three-way sample by metabolite by timepoint data array that we discussed at the start of this paper. This example is more subtle than the previous one, because all data entries may be expressed in the same measurement unit (e.g., number of ion counts in mass-spectrometry). Nevertheless, as mentioned in the Introduction, array-conditionality could be violated in this case, too, because of differences in instrumental response factors for the metabolites. As a consequence, it is possible that meaningful comparisons can only be made between data entries pertaining to the same metabolite, implying that this may be considered an example of lateral (metabolite-) slice-conditionality.

The third example turns out to be even more subtle. For this purpose, we again consider the three-way sample by metabolite by timepoint data. However, to rectify the metabolite-specific slice conditionality, we preprocess the data making use of instrument factors as obtained from calibration information (forgetting for a moment that this may be too elaborate in practice in case of hundreds of metabolites). At first sight, it may seem that now full array-conditionality is obtained: All values can now be interpreted in terms of concentrations. However, up to this moment, we have not yet considered the conceptual model of the biological system under study. It could, for example, be that all metabolites invoke a similar signalling response in a cell. From the point of view of the conceptual model, the subsequent signalling effect size may be the relevant aspect to consider in the comparison of data entries. To arrive at this information, an additional normalization would be needed.

The examples as listed above make clear that conditionality, in general, is a fairly tricky issue. Indeed, it involves: (a) measurement units and scales, (b) aspects of the experimental design and procedure that have been used in the data collection, and (c) the conceptual model of the system under study (which implies that conditionality is not an absolute issue that only depends on the data in themselves). Otherwise, it should be noted that the first aspect (measurement units and scales) implies that conditionality is inextricably bound up with the issue of transformational freedom.

Transformational freedom means that data can be subjected to some class of transformations, without loss of content-specific information. As an example, in the case of patient by clinical marker variable information, the variable pertaining to body temperature could be converted from centigrades to degrees Fahrenheit (or vice versa), without loss of any information.

Transformational freedom immediately relates to the concept of measurement level as introduced by [5]. Different measurement levels are typically associated with different classes of *permissible* transformations. For *nominal* scales, only identity represents meaningful information, and therefore any one-to-one transformation is permissible. For *ordinal* scales, only the rank order of numbers is relevant; this implies that all monotonic increasing transformations are permissible. On an *interval* level, beyond rank order, ratios of differences are meaningful (e.g., the 'difference between two body temperatures is twice as large as the difference between two other body temperatures', a statement that holds irrespective of whether temperature is expressed in centigrades or degrees Fahrenheit); as a consequence, linear transformations with a positive slope are permissible. For *ratio* scales, ratios are meaningful (e.g., 'the metabolite concentration in a first sample is twice as large as in a second sample'); on this level, linear transformation with positive slope and zero intercept are permissible. Finally, on an *absolute* level, the full numerical information is meaningful (which makes only the identity transformation permissible).

If one takes the measurement level issue serious, this may be fairly consequential, in that it places limitations on the statistics one may meaningfully employ [6]. More in general, one may expect the results of a meaningful data analysis to be insensitive to any permissible transformation of the data.

The measurement level issue is not free from controversy (for an overview of criticisms, see [7]). One of the stronger voices in the debate simply stated that 'Permission is not required in data analysis' [8].

For our argument, it is important to note that measurement level and transformational freedom may complicate the conditionality issue. Indeed, assuming three-way data, in case of some kind of slice- (resp. fiber-) conditionality, in principle different permissible transformations could be considered for different data slices (resp. data fibers). Moreover, in such a case, even measurement level (and, hence, the *family* of permissible transformations) could be considered to vary across data slices (resp. data fibers).

3.2. Lack of invariance

The conditionality obstacle to comparability pertains to cases in which comparisons of entries across the full data array are not meaningful. The type of obstacle to comparability that we will discuss in the present subsection is perhaps even more fundamental in nature: it pertains to whether comparisons *within* certain data slices or fibers are meaningful.

To understand this second type of obstacle, we start from the observation that subarrays of a multiway data array (e.g., slices and fibers of a three-way array) are characterized by constancy of an element within at least one data mode. As an example, a horizontal slice of a three-way data array consists of data entries that all pertain to one and the same element of the row mode (see also Fig. 3). As a second example, a horizontal fiber of a three-way array consists of data entries that all pertain to one and the same element of the row mode and one and the same element of the depth mode (see also Fig. 3).

Now, for comparisons between entries within a horizontal data slice to make sense, it is of key importance that, from the point of view of the conceptual model underlying the data, the meaning of the row mode element as associated with that slice is invariant across the full slice. From its part, for comparisons within a horizontal fiber to be meaningful, the meaning of both the row and depth mode elements as associated with that fiber should be invariant across the full fiber. Similar conditions can be formulated for the other types of slices and fibers.

The invariances as outlined above are also implicitly assumed in standard data-analytic modeling approaches. As an example, one may refer to the PARAFAC model with model Eq. (1). In this model, the meaning of each row mode element is represented by its corresponding row in the row mode component loading matrix $\mathbf{A}$. As such, it is invariant across the full horizontal data slice corresponding to the element in question.

To understand why the invariance assumption may be easily violated in data-analytic practice (without the researcher necessarily being aware of this), we revisit the example of the three-way sample by metabolite by timepoint data array as outlined at the beginning of the present paper. In this example, we take a closer look at the frontal slices, pertaining to single timepoints, or to vertical fibers as associated with a specific combination of a metabolite and a timepoint. Meaningful comparisons within such slices and fibers presuppose that the meaning of a timepoint is the same across all samples. Note that what is at issue here is the *biological* meaning of the timepoint, because physically speaking, the timepoint is obviously invariant. Stated differently, what is relevant in this case is the *biological time*. Suppose now that some of the samples pertain to blood whereas other ones pertain to urine of the same individual. Obviously, it is known that metabolites usually appear earlier in the blood. From the point of view of a conceptual model that takes into account the time lag between blood and urine, this could imply that the biological meaning of a timepoint is *not* invariant within frontal data slices and vertical data fibers. A less obvious example arises with

blood samples only, if those have been taken from different individuals at the same physical timepoints. As it is not clear whether the biological time for the different individuals is the same, also in this case the analysis of the data is not straightforward.

If the content-specific meaning of the element of some mode is not invariant across the elements of one of the other modes, this implies a major problem for comparability. This problem is fairly fundamental, because it implies that, whereas on a surface level the data look as if they have a fully crossed multiway structure, from the point of view of the conceptual model this is actually not the case. For instance, in the longitudinal metabolomics example, one could at first sight think that this example implies fully crossed sample by metabolite by timepoint data. However, if one takes into account that the biological times of samples pertaining to blood and urine samples might be translated into different physical times, this could imply that a different data structure, with timepoints being nested in samples, would be more appropriate.

4. Proposed solutions

Solutions that have been proposed so far to deal with lack of comparability can be ordered into two categories: Either they try to restore comparability through suitable transformations at the level of the data and/or at the level of the model, or they try to lower the comparability requirements by moving to a less demanding type of modeling. Below we will discuss these two types of proposed solutions more in detail.

4.1. Transformations

Attempts to restore comparability through suitable transformations can be organized on the basis of four types of distinctions:

- A first and important type of distinction pertains to whether one wishes to transform only on the basis of elements that are external from the point of view of the data, or rather that one wishes to consider transformations that are (fully or partially) data-based. External elements may include both a priori or theoretical concerns, and concerns that are based on data other than the actual data under study. As a first example, in case of multiway data that are expressed on scales that include a scale point that, on a priori or theoretical grounds, can be considered a neutral point, one might prefer to transform the data in terms of deviations from those neutral points. As a second example, in the metabolomics example that we launched at the beginning of the present paper, one could consider to deal with lack of comparability of the metabolites due to instrumental response factors by means of a transformation based on calibration information. This calibration information is to be distinguished from the actual sample by metabolite by timepoint data. As such, it can be considered *external* information. An example of a data-based transformation is that of autoscaling.
- Within the category of transformations that are (fully or partially) data-based, a second distinction can be drawn, depending on whether the transformations are carried out prior to the actual data analysis (which means that they come down to a preprocessing of the data in the strict sense), or rather that the transformations are estimated as a part of the actual data-analytic process. Furthermore, in the latter scenario, transformations may be considered on the level of the data $\mathbf{D}$, on the level of the reconstructed data $\hat{\mathbf{D}}$, or on the level of constituents of the reconstructed data (e.g., transformations of one of the component score matrices). Optionally, one could still consider a third moment for a transformation: *after* the actual data analysis (i.e., post-processing of the data-analytic output; for an example, see [9]); in the present paper we further leave this option aside.
- A third type of distinction pertains to the type of the transformations that one wants to consider. In this regard, one may first draw a distinction between local and global transformations. Local transformations can be defined as functions with single data entries as arguments. Linking up with [9], within the family of local transformations, one could distinguish between additive, multiplicative, and nonlinear transformations. (As, mathematically speaking, the class of all possible transformations is unbounded, the latter category of nonlinear transformations is very broad indeed, and includes both nonlinear monotonic transformations (with, e.g., logarithmic and monotonic spline transformations — including piecewise linear transformations as a special case), and all kinds of nonmonotonic transformations.) Global transformations are more involving types of transformations. Examples of such transformations include conversions into correlations or similarities, transformations into first-order difference scores[9], and spectral decompositions.
- Fourthly, for local transformations one may consider their level of specificity. A useful distinction in this regard is that between transformations on the level of the (observed or reconstructed) data array as a whole, and slice- (resp. fiber-) specific transformations that are allowed to vary across slices (resp. fibers). Examples of transformations on the level of the data array as a whole include a logarithmic transformation of all (observed or reconstructed) data entries, and a data centering based on the global array mean. Examples of more specific transformations include centering on the basis of slice- or fiber-specific means, monotonic transformations that are allowed to vary across slices or fibers, calculation of deviation scores from fiber- or slice-specific neutral points, transformations on the basis of fiber-specific calibration information, and slice- or fiber-specific transformations of component scores for the mode(s) that vary within the slices or fibers in question.

It may be useful to note that one may consider joint multiple local transformations for one and the same data set. Examples of such multiple transformations include a double centering based on both the row and column marginal means, and a fiber-specific centering along with a slice-specific scaling.

Below, we will consider more in detail two categories of data-dependent transformations that differ from one another with regard to the second type of distinction: preprocessing and transformation estimation as a part of the actual data-analytic process.

4.1.1. Preprocessing

In [9] no less than eight different reasons have been listed for preprocessing multiway data prior to the actual data analysis. At least three of these reasons pertain to 'facilitating' comparisons in some sense.

In [9] Harshman and Lundy further present a more in-depth discussion of several types of additive preprocessing (primarily centering) and multiplicative preprocessing (referred to as scaling). Both types of preprocessing are further considered on different levels of specificity (array, slice, and fiber), also taking into account the option of simultaneous multiple transformations. A summary and extension of a part of the discussion can be found in [10].

In the discussion, three different perspectives are important: (a) that of standard multilinear multiway models, such as the PARAFAC model of Eq. (1) with a standard loss function as in Eq. (2), (b) that of a standard multiway model with a weighted loss function, such as, for example,

$$\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K} w_i\left(d_{ijk}-\hat{d}_{ijk}\right)^2 = \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K} w_i e_{ijk}^2, \tag{3}$$

and (c) that of a standard multilinear multiway model extended with offset terms, such as,

$$d_{ijk} = \sum_{p=1}^{P} a_{ip}b_{jp}c_{kp} + \mu_i + e_{ijk} \tag{4}$$

(plus possibly other singly or doubly subscripted offset terms), with a standard loss function as in Eq. (2).

Three general results with regard to these three perspectives deserve a special mentioning:

- In case of standard multilinear models such as PARAFAC, an extended model that includes offset terms such as the model of Eq. (4) can be rewritten as a special case of its counterpart without offset terms (the reverse of course being trivially true as well). This relation, however, is primarily of theoretical importance only, as, in practice, a data analysis based on a model without offset terms may be less suitable to retrieve a model structure with offset terms (amongst other things, because of problems of overparameterization and identifiability).
- For a number of standard multilinear models, the minimization of a standard loss function as applied to multiplicatively preprocessed data can be shown to be equivalent to the minimization of a weighted loss function (such as in Eq. (3)) for the original data.
- In a number of cases, the estimation of the loading matrices of standard multilinear models extended with offset terms (such as the model of Eq. (4)) can be achieved through the fitting of the counterpart models without offset terms to an appropriately centered version of the data. This means that a sequential strategy consisting of first centering and subsequently fitting a multilinear model without offset terms may yield optimal estimates for a multilinear model with offset terms. It should, however, be noted that such a procedure: (1) does not yield unique estimates of the offset terms, (2) may provide centered estimates for some of the component loading matrices, (3) requires well-defined types of centering on correct levels of specificity (with inappropriate types of centering possibly being harmful for the data-analytic process). For more details on the equivalence as outlined above, the reader may consult [10,11].

As pointed out by [9], the relations (and in particular the equivalences) as outlined above may erroneously lead to the suggestion that a multilinear modeling of a data set that is subjected to an additive or multiplicative preprocessing leads to a solution that is structurally equivalent with a multilinear modeling of the raw data. This, however, is in general far from true. As such, subjecting data to an additive or multiplicative preprocessing may be very consequential for the subsequent data analysis.

4.1.2. Estimation of transformation(s) as a part of the data-analytic process

We consider three clusters of approaches that include a transformation estimation within the actual data-analytic process:

- A first cluster pertains to the estimation of multilinear models that include offset terms. An example of such a model has already been introduced above in terms of Eq. (4). This equation implies that:

$$\hat{d}_{ijk} = \sum_{p=1}^{P} a_{ip} b_{jp} c_{kp} + \mu_i, \tag{5}$$

  which makes clear that such models involve additive transformations ($+\mu_i$) on the level of the reconstructed data $\hat{\mathbf{D}}$. Moreover, as mentioned above, in the estimation of such models, the distinction between preprocessing and estimation during the actual model estimation is somewhat blurred, as in quite a few cases sequential strategies that include an appropriate preprocessing (viz., an appropriate type of centering) as a first step may constitute a viable estimation procedure for the loading matrices of multiway models extended with (singly subscripted) offset terms [11].
- A second cluster of approaches pertains to data situations in which the elements of at least one of the data modes take values on some dimension that is *external* to the actual data. Examples include multiway data in which one of the data modes pertains to different timepoints (as in the three-way sample by metabolite by timepoint data that we introduced at the beginning of the present paper). Other examples are data one mode of which pertains to wavelengths, or to elements that take a position on some underlying spatial dimension. Without loss of generality, in what follows we will call the externally quantifiable mode the time mode.
  In case of data that involve a time mode, one may consider extensions of standard multilinear models that include transformations of the component loadings for the elements of that mode, with these transformations differing depending on the elements of a mode (or of several modes) other than the time mode. Optionally, these transformations could be constrained to be the same for all components (which, in line with [12], can be called a synchronized component transformation).
  A representative family of models within this cluster is that of shifted factor analysis [13–15]. In case the third (or depth) mode is the time mode and the shifts are allowed to vary across the second (or column) mode, the shifted PARAFAC model is represented by the following equation:

$$d_{ijk} = \sum_{p=1}^{P} a_{ip} b_{jp} c_{(k + s_{jp})p} + e_{ijk}, \tag{6}$$

  with s_{jp} denoting the amount of time shift for component p in the slice defined by column j.
  A related family of models is that of warped factor analysis [16]. This family of models implies shape transformations of the profiles of component loadings across time, with these transformations differing depending on the elements of a mode other than the time mode. The warping transformations in question are obtained by a segmentation of the time range, by a mapping of the old segmenting nodes on new ones, and by a subsequent linear stretching or shrinking of the time segments between the nodes. Furthermore, as for the shifts, the warpings can optionally be constrained to be the same for all components. Again assuming that the third (or depth) data mode is the time mode and that the warpings are allowed to vary across the second (or column) mode, a warped variant of the PARAFAC model may look as follows:

$$d_{ijk} = \sum_{p=1}^{P} a_{ip} b_{jp} c_{(w_{jp}(k))p} + e_{ijk}, \tag{7}$$

  with w_{jp} denoting the warping of the time mode for the p^{th} component in the slice defined by column j. Note that Eq. (7) may be alternatively rewritten as:

$$d_{ijk} = \sum_{p=1}^{P} a_{ip} b_{jp} c_{(k + \tilde{w}_{jkp})p} + e_{ijk}, \tag{8}$$

  with $\tilde{w}_{jkp}$ denoting the warp for timepoint k (in the slice defined by column j in case of the p^{th} component). This rewriting makes clear that warps act as shifts that vary across the time mode (as appears from their additional subscript k).
  As already pointed at above, shifts and warpings are transformations on the level of the component loadings, rather than on the level of the observed or reconstructed data. Moreover, in the definition of shifts and warpings, the component loadings are considered as functions of the external quantification of the 'time mode', with shifts and warpings resulting from an operation on the input or argument of the functions in question. For example, in the shifted PARAFAC model of Eq. (6), the component loadings for the time mode, $c_{(k+s_{jp})p}$, can be considered functions, the first argument of which (i.e., k) underwent an additive transformation ($+s_{jp}$). (For a different approach with shifts operating on the output rather than on the input of the component loading

functions, see [9].) As such, in shifted and warped factor analysis, the transformations are based on both internal and external data information. Furthermore, regarding the type of transformation involved, on the level of the input of the component loading functions, the transformations can be considered as linear (resp. piecewise linear); yet, on the level of the output (i.e., the actual component loadings), the transformations can be considered as highly nonlinear.

The most important content-specific ground for invoking shifting or warping transformations is the need for restoring comparability by aligning the time mode for different data slices or fibers. To clarify this, we revisit the example of the three-way sample by metabolite by timepoint data array, with some of the samples pertaining to blood and other ones pertaining to urine. To synchronize the blood and urine data slices in terms of the biological time (which may require undoing the lag in objective time between both kinds of samples), one could consider the following variant of the shifted PARAFAC model of Eq. (6):

$$d_{ijk} = \sum_{p=1}^{P} a_{ip} b_{jp} c_{(k + s_{ij})p} + e_{ijk}, \tag{9}$$

with s_{ij} denoting the amount of time shift in the data fiber pertaining to (blood or urine) sample i for metabolite j (which is synchronized across components). The shift parameter s_{ij} now has indices i and j, as the shift may depend on the specific biological compartment i and on the metabolite j [17].

As a second example, to synchronize the blood data obtained from different persons at the same timepoints, one may consider using

$$d_{ijk} = \sum_{p=1}^{P} a_{ip} b_{jp} c_{(k + s_i)p} + e_{ijk}, \tag{10}$$

where the shift parameter s_i is now indexed by i, as the shift depends on the individual i. Otherwise, the shift not depending on the metabolite implies the assumption that all metabolites are shifted between individuals i by the same amount. This may be an oversimplification and, hence, in practice one has to test whether this assumption holds.

- A third cluster of approaches involves so-called optimal scaling [18]. Optimal scaling pertains to transformations of the actual data (rather than of the reconstructed data or of model constituents such as component loadings). It immediately links up with the issues of conditionality, transformational freedom, and measurement level as outlined in Section 3.1. In optimal scaling approaches, a loss function of the following type is to be optimized:

$$\sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} \left[f\left(d_{ijk}\right) - \hat{d}_{ijk} \right]^2, \tag{11}$$

with the optimization being done over all model parameters of the multilinear model under study and over all permissible transformation functions f. As discussed in Section 3.1, the family of permissible transformation depends on the measurement level that is being considered for the data (with, e.g., for ordinal data all monotonic increasing transformations being permissible). Depending on the conditionality of the data, the optimal scaling function f may further be allowed to be constant or to vary. In particular, array-conditional data are associated with a single transformation or optimal scaling function f. However, in case of slice- or fiber-conditional data, one should allow the optimal scaling function to vary across data slices (resp. fibers); in symbolic terms, this can be denoted by providing the function f with a single or double subscript. As an example, if one would consider a sample by metabolite by timepoint data array as metabolite-conditional (which implies that comparisons of data entries are only meaningful within and not across metabolites), one could consider to estimate a multiway model extended with optimal scaling, making use of the following loss function:

$$\sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} \left[f_j\left(d_{ijk}\right) - \hat{d}_{ijk} \right]^2, \tag{12}$$

One should finally remember that, in case of slice- or fiber-conditional data, the measurement level (and, hence, the family of permissible optimal scaling transformations) may also be allowed to vary across data slices (resp. fibers).

4.2. Adjusted modeling that requires less comparability

Quite a different way to deal with problems of lack of comparability consists of moving to a different type of modeling with lower comparability requirements. To illustrate, we revisit the example of a three-way sample by metabolite by timepoint data array, with a set of samples that are the same in nature (e.g., measurements in blood) obtained from different individuals. A standard multilinear multiway model for these data such as the PARAFAC (or PARAFAC1) model of Eq. (1) presupposes a mechanism underlying the data that is based on invariant characteristics of the timepoints, as represented by the timepoint loadings $c_{kp}, p = 1,\ldots,P$. However, it may be questionable whether the biological meaning of timepoints is invariant across all individuals. To deal with this comparability problem, one could consider moving to a PARAFAC2 model [19], with the following model equation:

$$d_{ijk} = \sum_{p=1}^{P} a_{ip} b_{jp} c^{i}_{kp} + e_{ijk} \tag{13}$$

(with in addition an identifiability constraint on the matrices $\mathbf{C}^i$, which we leave here further aside). Obviously, by making the loadings c_{kp} of timepoint k depend on the sample or individual i, the comparability problem is dealt with, in that the mechanism underlying the data is no longer assumed to depend on characteristics of the timepoints that are invariant across individuals. An insightful application in which comparability problems are dealt with by replacing a (four-way) PARAFAC1 model by a (four-way) PARAFAC2 model can be found in [20].

A similar move towards modeling that implies less comparability requirements is exemplified by replacing a Tucker3 model by a PCA-SUP or Tucker1 model (see, e.g., [21]). In all such cases, the data under study apparently have a fully crossed three-way structure. Yet, in fact in the modeling they are dealt with as if one of the modes (in our example: the timepoint mode) is *nested* in one of the other modes (in our example: the sample or person mode).

An analogous approach can be found in the family of models for multivariate curve resolution. This family has been developed to represent spectroscopic measurements taken over time on chemical systems [22]. In these models, the time direction is considered nested in the repeated batch sampling mode (with the model parameters being calculated by, e.g., imposing kinetic equations in the time direction [23]).

5. Evaluation of proposed solutions

5.1. Transformations

5.1.1. External bases for transformation

We start by considering possible external bases for transformation, under the form of a priori conceptual/theoretical information or of empirical information outside the actual data (such as calibration

information). It should be clear that, if such external information is available, and if this information is relevant from the point of view of the conceptual model of the system that generated the data, then one should definitely use it to guide the transformation process. Otherwise, cases in which such information is available may also give rise to an interesting thought exercise: Suppose one would ignore for a moment the information in question. For the data analysis, one then may consider to rely on internal data-based transformation procedures, either under the form of data preprocessing or under the form of a data-analytic process that includes a transformation estimation. A key question then reads whether such procedures would allow the researcher to recover the results of a data-analytic endeavor that does take the external information into account. It is rather easy to come up with examples in which this is not the case. Obviously, such examples cast at least some doubt on the validity of internal data-based transformation procedures.

5.1.2. Internal data-based transformation procedures: surface level

Internal data-based transformation procedures (prior to or within the actual data-analytic process) can be evaluated on a *surface level* and on a *depth level*. On a surface level, one may first note that transformations are in general fairly consequential. Next, one may wonder whether the consequences of the transformations are desirable or not. Desirable consequences include the fact that appropriate types of transformations may discard unwanted sources of variance. As an example, a multilinear modeling of raw multiway data may be guided to a strong extent by main effects as present in the data. If this is undesirable, preprocessing the data with suitable procedures of centering and/or estimation of a multilinear model that includes one or more singly subscripted offset terms may provide a neat way out.

A second desirable consequence pertains to situations of transformational freedom, that is, situations in which the data can be subjected to some class of permissible transformations that do not alter content-specific information. In such cases, internal data-based transformation procedures may remove, at least in part, arbitrariness in the modeling output due to the choice of a particular quantification of the data. As an example of this, one may consider a series of variables that are considered to be measured on interval scales (which implies that, without loss of information, those variables may be subjected to any linear transformation with a positive slope). In such a case, a variable-conditional autoscaling would yield preprocessed data, for which the results of any subsequent data analysis would not depend on the actual quantification of the original raw data. Another example of a procedure to remove transformational freedom is given by all methods relying on optimal scaling such as the ALSCOMP procedure as proposed in [18] for a multiway situation. Inspection of the loss function (11) that is optimized in such a procedure makes clear that the modeling output necessarily remains the same, irrespective of the particular permissible quantification of the raw data that is taken as a starting point. (One may note that the fact that the optimal scaling transformation f operates on the data $\mathbf{D}$ rather than on the reconstructed data $\hat{\mathbf{D}}$ plays a key role in guaranteeing invariance under the choice of a permissible quantification of the data.)

Less desirable aspects and consequences of transformations include the fact that they may introduce unwanted variation. As an example, in the case of patient by clinical marker variable data, autoscaling each of the variables may 'blow up' the (error) variance of variables with regard to which the patients do not meaningfully differ.

Another less desirable aspect, especially for methods in which transformations are estimated as a part of the data-analytic process, is more technical in nature. Indeed, the estimation involved in such methods is fairly complex. As a consequence, the methods in question may, for instance, be much more vulnerable to local optima problems [9].

5.1.3. Internal data-based transformation procedures: depth level

Beyond concerns on a surface level, internal data-based transformation procedures raise much more fundamental questions: if the data suffer from problems on the level of conditionality or invariance, do internal data-based transformations truly remedy for these? If some raw data entries cannot be meaningfully compared, do these procedures effectively restore comparability? Do the procedures (e.g., the procedures involving optimal scaling) yield, indeed, quantifications of the data that are meaningful (and meaningfully comparable) as such (and, hence, that can be situated on an interval or ratio scale level)? Do shifting and warping procedures truly remedy for a lack of timepoint invariance, in terms of a correct time mode alignment?

It should be emphasized that the questions as listed above are far from trivial or easy. To illustrate, we first revisit the example of a two-way patient by clinical marker variable data set. One may perhaps wish to rectify the lack of comparability of the different markers (which are expressed in different measurement units), by autoscaling each of the variables. However, when thinking through this example (including the possibility that the variables may considerably differ in the true amount of between-patients heterogeneity) there is no strong basis at all for claiming full comparability (or matrix-conditionality) of a columnwise autoscaled transformation of these data.

Similarly, one may wonder whether procedures of optimal scaling do yield, indeed, transformed data on an interval or ratio level that can be meaningfully compared in all possible respects. One of the problems in this regard is that there are many widespread misconceptions about the measurement level of data, with many people erroneously believing that measurement level is an absolute and unconditional issue that exclusively pertains to the input of the data-analytic process. Yet, as convincingly argued in [24], claims about a measurement level can only be justified provided an almost perfect fit of a model to the optimally scaled data, and provided an equivalent result with a modeling under the assumption of a lower measurement level. This clearly implies that measurement level statements: (a) constitute a relative issue, which depends on the model chosen (in conjunction with optimal scaling), (b) constitute a conditional issue, the conditions pertaining to (almost) a perfect model fit and to equivalence between different modeling outcomes, (c) pertain, at least to a large extent, to the *output* rather than the input of the whole modeling endeavor. Beyond all this, to arrive at transformed data entries that can be meaningfully compared in all possible respects, not only the data-analytic model under study but also the optimal scaling transformation should be justifiable from the point of view of the conceptual model of the system that generated the data. The latter is perhaps an even more critical issue.

A similar concern could also be expressed about methods involving shifts or warpings. For such methods to truly remedy for a lack of timepoint invariance, the shifts or warpings (as well as the actual factor-analytic model) should be grounded in the conceptual model of the data-generating system.

5.2. Adjusted modeling that requires less comparability

Rather than trying to rectify comparability problems through suitable transformations, one could simply move to a different type of modeling with lower comparability requirements. Such an approach could be justified provided it meets what the researcher really cares about, and provided that the new type of data-analytic model is a correct implementation of the underlying conceptual model. Furthermore, in selecting this type of approach, one should at least be fully aware that it implies abandoning attempts to restore certain aspects of comparability or synchronicity, and to retrieve invariant characteristics of one of the data modes under study.

6. Concluding remarks

This paper focused on a key issue in multiway data analysis: the issue of comparability. Comparability pertains to the content-specific meaningfulness of the numerical values of data entries and of their comparisons.

Comparability is implicitly required in many methods for multiway data analysis, as such methods often rely on a least squares loss function that entails a summation of residuals across the full multiway data array. Otherwise, one may note that this also holds true if the methods in question are used as mere techniques of data reduction. If the researcher wants to go beyond such a mere data reduction and cares about examining his data on the basis of a conceptual model of the data-generating system (which should ultimately lead to a data-analytic model and parameter estimates that embody well-interpretable, content-specific data mode characteristics), then comparability requirements are even much more stringent.

However, in data-analytic practice there are major obstacles to comparability (which, unfortunately, are erroneously being overlooked too often). Those can be roughly grouped under two headings. To clarify this we consider the comparison of two data entries (e.g., d_{ijk} and $d_{i'jk}$). A first group of obstacles pertains to the subscripts that differ across the two entries in question (in our example, i and i'). A meaningful comparison of the entries under study could be hampered by conditionality aspects (including measurement scale and measurement level aspects) involving in our example elements i and i' of the row data mode. A second group of obstacles pertains to the subscripts that do not differ across the two data entries (in our example, j and k). For the comparison of the data entries to be meaningful, one may want the meaning of the j^{th} element of the column mode and the k^{th} element of the depth mode to be invariant across all elements of the row mode.

The obstacles as outlined above are ubiquitous in data-analytic practice. As such they already occur quite often in the case of two-way data. In a multiway data setting, however, the problems are typically more severe, as many more kinds of comparisons and invariances play a role here. The situation is perhaps even more problematic in cases with multiset data, because there both within- and between-set comparisons are at issue [25].

Several obstacles to comparability have originally been pointed at in psychometrics. Those include the aspects of conditionality [3] and measurement level [5]. This is rather easy to understand if one considers psychological data, such as preference rankings by participants of objects (e.g., paintings or holiday destinations) as collected in a two-way participant by object data matrix. When taking a superficial glance at this type of data, one can easily be tempted to classify them as row- (or participant-) conditional (implying that meaningful comparisons of rank numbers can only be made within a participant and not across participants); also, one could consider the data to be measured on an ordinal level (in that monotonic increasing transformations of the rank numbers would not affect the content-specific information). However, in psychometrics, obstacles to comparability also occur in far less transparent or obvious settings. Moreover, in the present paper, we have shown that comparability problems are no less frequent in areas such as chemometrics and bioinformatics (see, e.g., the recurring longitudinal metabolomics example), notwithstanding the fact that one might expect the contrary for areas in which researchers may rely on more objective types of measurement.

In this paper, we further reviewed a number of solutions that have been proposed thus far to deal with comparability problems. On a surface level, pros and cons of those proposed solutions are rather straightforward. However, deeper questions on whether the solutions in question do restore comparability and invariance, indeed, are much less trivial. All in all, whether the solutions can be expected to work can only be answered upon a careful reflection about the data collection, about which conceptual model one wants to use for the data-generating system, and about how this conceptual model relates to the actual data-analytic model (including all possible transformations one is willing to include before or during the actual data-analytic process). Furthermore, interpretations on the level of the conceptual model can only be expected to work provided a very good fit of the data-analytic model to the actual data.

In the discussion on measurement level and permissible transformations, one of the leading commentators has argued against the introduction of 'permissions' in data analysis [8]. Taking into account the many misconceptions and unclarities surrounding the concept of measurement level, this is perhaps not the worst possible advice. However, no researcher should ever be given a permission to go for a 'mindless' data analysis, that is, a data analysis without a careful reflection about what one really cares about. Such a reflection should further include all aspects of the data-analytic process: the method and procedures used in the data collection, the conceptual model of the data-generating system under study, the mathematical structure of the data-analytic model, the loss function that is to be optimized in the data analysis, and the data and modeling aspects that are to be included in model selection and in the evaluation of model quality and goodness of fit. Finally, the need for a careful reflection does not mean that fully-fledged conceptual and data-analytic models should already be available at the beginning of a data-analytic process. Neither does it mean that data-analytic processes are inherently linear, nor that the only worthwhile types of data analysis are confirmatory or hypothesis testing like in nature. Obviously, insights into conceptual and data-analytic models can grow during inherently cyclic data-analytic movements, fueled by enduring reflections on what one really cares about as a data analyst.

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