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Solving the sign indeterminacy for multiway models

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Bilinear and multilinear models such as principal component analysis and PARAFAC have intrinsic sign indeterminacies. For example, any loading vector can be multiplied by −1 if another vector of that particular component is also multiplied by −1 without affecting the loss function values. This sometimes causes problems, for example, with respect to interpretation. In this paper, a method is developed to fix the sign indeterminacy for the PARAFAC, Tucker3 and PARAFAC2 models. Copyright © 2013 John Wiley & Sons, Ltd.

Keywords: sign flip; tensor models; PARAFAC; Tucker3; PARAFAC2

1. INTRODUCTION

Latent variable models such as principal component analysis (PCA) [1–3], PARAFAC [4,5] and Tucker [6,7] have intrinsic sign indeterminacies. For example, in a PCA model, it holds that the scores (**T**) and loadings (**P**) are found to minimize the least squares loss function $\|\mathbf{X}-\mathbf{T}\mathbf{P}^T\|_F^2$. This loss function is identical to $\|\mathbf{X}-(-\mathbf{T})(-\mathbf{P}^T)\|_F^2$, and hence, the score matrix can be exchanged with $-\mathbf{T}$ as long as the loading matrix is replaced with $-\mathbf{P}$. Mathematically, there is no way to distinguish between the two solutions.

In a two-way model, changing the sign of, for example, the score vector of component three is explicitly countered by having to change the sign of the corresponding third loading vector. Samples that have high positive scores on this original component have high values on the variables with high loading elements. This interpretation is unchanged, even when signs are switched, so the sign indeterminacy is of moderate consequence for a two-way model. In [8], a method was developed to assign meaningful signs to scores and loadings in PCA models. In this paper, these results are further developed to allow a similar sign correction of common multiway models.

In a PARAFAC model, it is also possible to change the sign of say the first column of the first mode component matrix **A** ($\mathbf{a}_1$), and it must be countered by changing the sign of either the corresponding second mode loading vector, $\mathbf{b}_1$, or the third mode loading vector, $\mathbf{c}_1$. Hence, for a one-component PARAFAC model, it holds that this component can consist of the following vectors:

$$(\mathbf{a}_1,\mathbf{b}_1,\mathbf{c}_1),(-\mathbf{a}_1,-\mathbf{b}_1,\mathbf{c}_1),(-\mathbf{a}_1,\mathbf{b}_1,-\mathbf{c}_1),\text{or }(\mathbf{a}_1,-\mathbf{b}_1,-\mathbf{c}_1)$$

Any of these representations of the component will have the same loss function value and are hence equally valid from a mathematical point of view.

For data such as many kinds of spectroscopy, the signs are easy to deduce from the appearance of the components, because underlying spectra, concentrations or time profiles are positive. In other situations though, there is no intrinsic convention that can help guide the appropriate choice of signs.

In 2008, the sign problem for PCA was suggested to be resolved using an assumption that the "natural" sign is the one that leads to a component that points in the direction where the majority of the data are pointing [8]. The basic premise of this approach is hinted at in Figure 1.

In this paper, similar approaches will be developed for PARAFAC, Tucker3 and PARAFAC2 models. In the following, we will use standard notation as given by Kiers [9]. Furthermore, residuals are excluded in all equations throughout, as the residuals are immaterial for the points made here.

1.1. Theory

1.1.1. PARAFAC

In PARAFAC, sign indeterminacies arise in the low-rank trilinear model because

$$\mathbf{X}_k=\mathbf{A}\mathbf{D}_k\mathbf{B}_k^T=\mathbf{A}\mathbf{S}_1\mathbf{S}_3\mathbf{D}_k\mathbf{S}_2\mathbf{B}_k^T,\text{for } k=1,\ldots,K$$

where $\mathbf{S}_1$, $\mathbf{S}_2$ and $\mathbf{S}_3$ are diagonal matrices with +1 or −1 on the diagonal. Together, they fulfill that $\mathbf{S}_1\mathbf{S}_2\mathbf{S}_3=\mathbf{I}$. Hence, the model given by **A**, **B** and **C** can be replaced by a model given by $\mathbf{A}\mathbf{S}_1$, $\mathbf{B}\mathbf{S}_2$ and $\mathbf{C}\mathbf{S}_3$ without changing the loss function. This extends without problems to PARAFAC models of an order higher than three.

To determine the appropriate sign, it is sufficient to consider one component at a time. The contribution from other components can be removed from the data before the sign of any given component is assessed [8].

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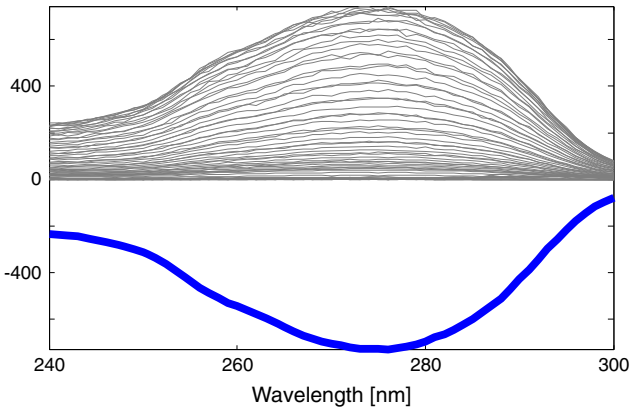

Figure 1. A set of spectra (thin lines) modeled by a one-component principal component analysis model. The first loading vector (estimated using the built-in function SVD in MATLAB R2011b) is shown with a thick line (scaled). It is apparent that the loading has a direction opposite to the majority of the data. Switching the sign of the loading (and the corresponding score) will give a model that is in better accordance with the data.

When the appropriate sign, for example, for the first mode component, is assessed, the PARAFAC model is re-expressed as a bilinear model

$$\mathbf{X}_{\text{unfold}} = \mathbf{a}\mathbf{z}^T$$

where $\mathbf{a}$ is the component (column of $\mathbf{A}$) currently considered and $\mathbf{z}$ is the Khatri–Rao product of the corresponding columns of $\mathbf{B}$ and $\mathbf{C}$. $\mathbf{X}_{\text{unfold}}$ is the three-way array unfolded/matricized appropriately. The vector $\mathbf{a}$ is normalized. For each column of $\mathbf{X}_{\text{unfold}}$, the inner product with $\mathbf{a}$ is calculated, squared and multiplied with the sign of the inner product as was suggested in the original PCA sign correction approach [8]. If a vector is in the same direction as $\mathbf{a}$ (corrected for the size), then this number is large and positive, and if it points in the opposite direction, then the number is negative. The sum of all numbers indicates how strongly $\mathbf{a}$ is in the same or opposite direction as the majority of the data,

$$s_{\mathbf{a}} = \sum_{j=1}^{J} \text{sign}\left(\mathbf{a}^T\mathbf{x}_j\right)\left(\mathbf{a}^T\mathbf{x}_j\right)^2 \quad (1)$$

where $\mathbf{x}_j$ is the jth column of the matricized array. The same procedure is repeated in each mode, giving a preferred sign for the component in each mode as well as a magnitude of *how* preferred the sign is.

If the number of negative signs is even, then the signs of each mode s_1, s_2 and s_3 will have a combined product of 1, and the signs of component vectors can hence be changed accordingly without changing the loss function. For example, if both $\mathbf{a}_1$ and $\mathbf{b}_1$ of component one has a negative s value, but $\mathbf{c}_1$ does not, then $\mathbf{a}_1$ is replaced with $-\mathbf{a}_1$ in the model and likewise for $\mathbf{b}_1$. As the product of $-\mathbf{a}_1$, $-\mathbf{b}_1$ and $\mathbf{c}_1$ remains the same as that of $\mathbf{a}_1$, $\mathbf{b}_1$ and $\mathbf{c}_1$, the model is unchanged.

If the number of negative signs is odd, the magnitudes are used to decide which one of the signs should be disregarded. The vector that has the sign with the lowest associated magnitude is modified opposite to what the sign suggests, thus making the product of signs equal to 1. Conflicting numbers of negative signs occur, for example, when data are centered, because then the direction in the centered mode can become arbitrary (yet of small magnitude). For more information on the basic procedure, please consult Bro *et al*. [8].

1.1.2. *Tucker3*

In essence, the preceding section defines how to assign proper signs for the PARAFAC model. Next, the Tucker3 model is considered. The Tucker3 model is a complicated model to explore and visualize because of the core array. Essentially all vectors in one mode interact with all the vectors in all other modes. This makes it impossible to visualize all modes of a Tucker3 model simultaneously as also described by Kroonenberg in his work on so-called joint plots [10]. It also makes it impossible to rigorously define a preferred overall direction/sign of a vector because any one-component vector can have different preferred directions depending on interactions in the other modes. Hence, a generic sign convention for Tucker3 will have to be somewhat ad hoc. One possible and feasible solution can be to focus on models that have approximately superdiagonal cores. Such rotated models can be simpler to interpret *if* the rotated model does indeed end up having an approximately superdiagonal core [11,12]. In such cases, we will advocate that the model be interpreted as a PARAFAC model disregarding the off-superdiagonal core elements when defining appropriate signs of components. That way, the signs of the components are switched by solely reflecting the interactions of vectors in different modes with similar component number.

A slightly more general solution is also developed. This approach can be used whenever the model is *not* interpreted as a PARAFAC model; that is, when the user also pays consideration to off-superdiagonal elements of the core in the interpretation. This method is also the one we have implemented in the software associated with this paper, but the "PARAFAC approach" is of course still viable. The general procedure proceeds as follows. Assuming at first that the core array has no preferred sign, the sign of loading vectors in each mode can be assigned independent of all the other modes because any sign switch in one-component matrix can be countered by a sign switch of the core.

The data to use for calculating the sign for a given vector are found by subtracting the remaining components. This means using all components in the other modes and using all but the given component in the mode of interest and the corresponding core array. This can be exemplified as follows. Assume that the sign of the fth component in mode one is sought. The Tucker3 model of the three-way array is given by the components in $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ and the core array $\mathbf{G}$. To remove the influence of remaining components, the model from those is subtracted as

$$\mathbf{X}_{\text{res}} = \mathbf{X} - \mathbf{A}_f\mathbf{G}_f\left(\mathbf{C}\otimes\mathbf{B}\right)^T \quad (2)$$

Here, $\mathbf{X}$ is the matricized three-way array and $\mathbf{A}_f$ is the first mode component matrix with column f excluded. The matrix $\mathbf{G}_f$ is the matricized core array where the fth horizontal slab has been excluded. The residual matrix $\mathbf{X}_{\text{res}}$ now contains the part of the original data that the fth column of $\mathbf{A}$ is modeling. Hence, the part of the Tucker3 model pertaining to that column can be written as

$$\mathbf{X}_{\text{res}} = \mathbf{a}_f\mathbf{z}_f^T + \mathbf{E} \quad (3)$$

where $\mathbf{a}_f$ is the fth column of $\mathbf{A}$ and $\mathbf{E}$ is the original residual array of the Tucker3 model. The vector $\mathbf{z}_f$ is defined by

$$\mathbf{z}_f = \mathbf{g}_f(\mathbf{C}\otimes\mathbf{B})^T \quad (4)$$

where the vector $\mathbf{g}_f$ is the vectorized fth horizontal slab of the core array.

Using the model representation in Equation (3), we can determine the appropriate sign of the fth column of $\mathbf{A}$ from Equation (1).

If the sign of column f is switched in $\mathbf{A}$, then correspondingly, the fth horizontal slab of the core array is multiplied by -1. With this approach, all vectors in all component matrices point in a preferred direction, all other things being equal. It may happen, though, that some core elements are negative, and we argue that in interpreting a Tucker3 model, it is most natural that core elements are positive. This can be compared with having negative singular values in a singular value decomposition. Although mathematically feasible, a positive value is more natural. It is not necessarily possible to transform any Tucker3 model to have all core elements positive. Rather than attempting this, we investigate only the largest core elements. Starting with the largest (negative) core element, the sign of this is switched by looking at the three vectors in each mode that it reflects. Assume that the core element is element (i, j, k), then the magnitude of s for the corresponding vectors $\mathbf{a}_i$, $\mathbf{b}_j$ and $\mathbf{c}_k$ is assessed according to Equation (1). Each of these three vectors has been sign corrected as outlined earlier, but the corresponding (large) core element is negative. It is therefore suggested to switch the sign of one of these three vectors that has the smallest value of s. This way, the largest combinations of core elements will end up having a "natural" core sign. This defines the sign convention for Tucker3.

1.1.3. PARAFAC2

Finally, the PARAFAC2 model is considered. This is, by far, a more complicated model to deal with. The PARAFAC2 model can be written as

$$\mathbf{X}_k = \mathbf{A}\mathbf{D}_k\mathbf{H}^T\mathbf{P}_k^T = (\mathbf{A})\left(\mathbf{D}_k\mathbf{H}^T\mathbf{P}_k^T\right) = \mathbf{A}\mathbf{G}_k^T{}^T, \text{for } k = 1,\ldots,K$$

which implies that the concatenated frontal slabs can be written as

$$[\mathbf{X}_1\mathbf{X}_2\cdots\mathbf{X}_K] = \mathbf{A}[\mathbf{G}_1\mathbf{G}_2\cdots\mathbf{G}_K]^T$$

This is a bilinear model, and the sign ambiguity within the product of $\mathbf{D}_k$ and $\mathbf{P}_k$ is essentially eliminated in this representation because only their product appears (inside $\mathbf{G}_k$). From this bilinear model, the overall sign of $\mathbf{A}$ and the concatenated matrix can be determined using the two-way sign correction approach described in Equation (1) [8]. This also extends to higher-order PARAFAC2 models, where instead of $\mathbf{A}$, the Khatri–Rao product of all but the two "special" modes would take the position of $\mathbf{A}$. Because the sign of $\mathbf{A}$ is then fixed, each slab, $\mathbf{X}_k$, can now be assessed using

$$\mathbf{X}_k = (\mathbf{A}\mathbf{D}_k)\left(\mathbf{H}^T\mathbf{P}_k^T\right) = (\mathbf{A}\mathbf{D}_k)\mathbf{S}_k\mathbf{S}_k\left(\mathbf{H}^T\mathbf{P}_k^T\right), \text{for } k = 1,\ldots,K$$

where $\mathbf{S}_k$ is a diagonal matrix with $+1$ or -1 on the diagonal. We can further develop this as

$$\mathbf{X}_k = (\mathbf{A}\mathbf{D}_k)\mathbf{S}_k\mathbf{S}_k\left(\mathbf{H}^T\mathbf{P}_k^T\right) = (\mathbf{A}\mathbf{D}_k\mathbf{S}_k)\left(\mathbf{S}_k\mathbf{H}^T\mathbf{P}_k^T\right), \text{for } k = 1,\ldots,K$$

Because the matrix $\mathbf{S}_k$ is specific to k, we cannot apply $\mathbf{S}_k$ to $\mathbf{H}$. This would change $\mathbf{H}$ and hence invalidate the model of other slabs. However, it can be shown that

$$\mathbf{S}_k\mathbf{H}^T\mathbf{P}_k^T = \mathbf{H}^T\mathbf{M}_k\mathbf{P}_k^T$$

where $\mathbf{M}_k = \mathbf{H}^T + \mathbf{S}_k\mathbf{H}^T$ because it follows that $\mathbf{H}^T\mathbf{M}_k = \mathbf{H}^T(\mathbf{H}^T + \mathbf{S}_k\mathbf{H}^T) = \mathbf{S}_k\mathbf{H}^T$ because $\mathbf{H}$ is a square and full-rank matrix per definition. Hence, we can sign correct $\mathbf{P}_k$ using $\mathbf{M}_k$ instead of $\mathbf{S}_k$. With this, the preferred sign for each pair of $\mathbf{P}_k$ and $\mathbf{D}_k$ can be determined and corrected. Note that the PARAFAC2 model is quite special in that each element of the diagonal of $\mathbf{D}_k$ can switch sign independently because of $\mathbf{P}_k$. This means that each and every element of the loading matrix $\mathbf{C}$ can change sign independently of all others. Also note that we do need to obtain the appropriate signs of the columns of $\mathbf{P}_k$ (and $\mathbf{H}$). Even though only the product of the two appear in the actual PARAFAC2 model, the correct signs of $\mathbf{H}$ are needed to find the appropriate signs of the remaining parameters.

With the sign of $\mathbf{C}$ fixed, there is still a potential sign indeterminacy within $\mathbf{P}_k\mathbf{H}$ because $\mathbf{P}_k\mathbf{H} = \mathbf{P}_k\mathbf{S}\mathbf{S}\mathbf{H}$. Notice that $\mathbf{S}$ is common to all slabs. We take a pragmatic approach and determine the appropriate sign for each slab as

$$\mathbf{X}_k = \mathbf{A}\mathbf{D}_k\mathbf{H}\mathbf{S}_k\mathbf{S}_k\mathbf{P}_k^T, \text{for } k = 1,\ldots,K$$

Subsequently, the most abundant sign is chosen by using the sign of the sum of all $\mathbf{S}_k$.

Thus, having fixed the sign ambiguity of the $\mathbf{P}_k$ matrices, we now correct the rest of the model parameters. For higher-order models, it may be necessary to express the model as a PARAFAC model given the fixed $\mathbf{P}_k$ matrices. Assuming a higher-order model where components of several modes are held as a Khatri–Rao product matrix [13] in $\mathbf{A}$, a model of the slabs $\mathbf{X}_k\mathbf{P}_k$ can be expressed as a PARAFAC model:

$$\mathbf{Y}_k = \mathbf{X}_k\mathbf{P}_k = \mathbf{A}\mathbf{D}_k\mathbf{H}^T\mathbf{P}_k^T\mathbf{P}_k = \mathbf{A}\mathbf{D}_k\mathbf{H}^T, \text{for } k = 1,\ldots,K$$

From this, the signs within the several modes in $\mathbf{A}$ (refer to earlier discussion) can be determined by using the sign fix approach of an ordinary PARAFAC model. Hence, all signs are thereby fixed.

2. RESULTS

To verify that the sign correction is meaningful, a few examples are given. One example on a Tucker model is given and two examples focusing on the PARAFAC2 model. The PARAFAC corrections are more straightforward extensions of the original sign correction of [8], so these are not further discussed here.

For exemplifying Tucker sign corrections, we analyzed a data set that describes the average daily amount of pollen for 40 weeks (first mode) for 16 plant families (second mode) during 5 years (third mode) in an area close to Tortona, Piedmont, Northern Italy [14]. The weeks taken into account go from Week 6 (mid-February) to Week 45 (beginning of November).

The 16 families are the following: Betulaceae, Corylaceae, Cupressaceae–Taxaceae, Fagaceae, Oleaceae, Pinaceae, Salicaceae, Chenopodiaceae–Amaranthaceae, Compositae, Graminaceae, Plantaginaceae, Polygonaceae, Urticaceae, Alternaria, Cladosporium and others + nonidentified.

The years covered are 2006–2010. For the final Tucker3 model, the number of components chosen was two in the first mode, two in the second mode and one in the third mode. The model is rotated to be superdiagonal in the 2×2 plane of the core, and this is perfectly achievable when the last mode

has only one component. Hence, components can be compared across modes. That is, score one in mode one is only related to score one in mode two and likewise for Score 2. After sign correction, the loading plots are as shown in Figure 2.

As opposed to the "original" orientation in the model, the sign correction allows us to have a direct joint interpretation of the loading plots. The period of pollination of each family can be easily seen (e.g., Salicaceae, Cupressaceae, Betulaceae and Corylaceae in spring; Fagaceae, Graminaceae and Polygonaceae in summer; and Compositae, Cladosporium and Alternaria in autumn), for example, in 2010, the spring pollination was slightly larger than that in 2008 and 2009.

For an example of sign correcting a PARAFAC2 model, a data set of 44 red wine samples is used. The volatiles of the samples were collected from 10 mL of each wine on a Tenax-TA trap. The trapped volatiles were desorbed using an automatic thermal desorption unit and transferred to a gas chromatography (GC) system (HP 6890 GC). The GC was equipped with a mass spectrometric detector operating in the electron ionization mode at 70 eV. More experimental details can be found in [15].

An example of a typical PARAFAC2 model from a part of the elution time is shown in Figure 3. A three-component unconstrained PARAFAC2 model seems to be appropriate, but several loadings are turned upside down. This is readily seen in

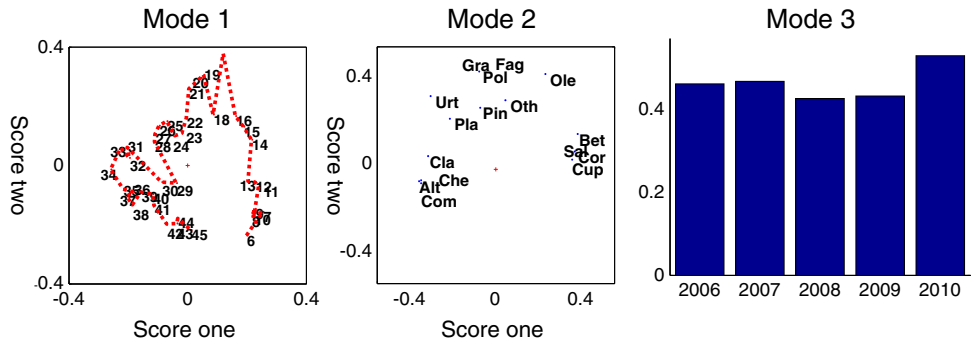

Figure 2. Sign-corrected scores and loadings of a Tucker3 model of pollen data with a diagonal core array.

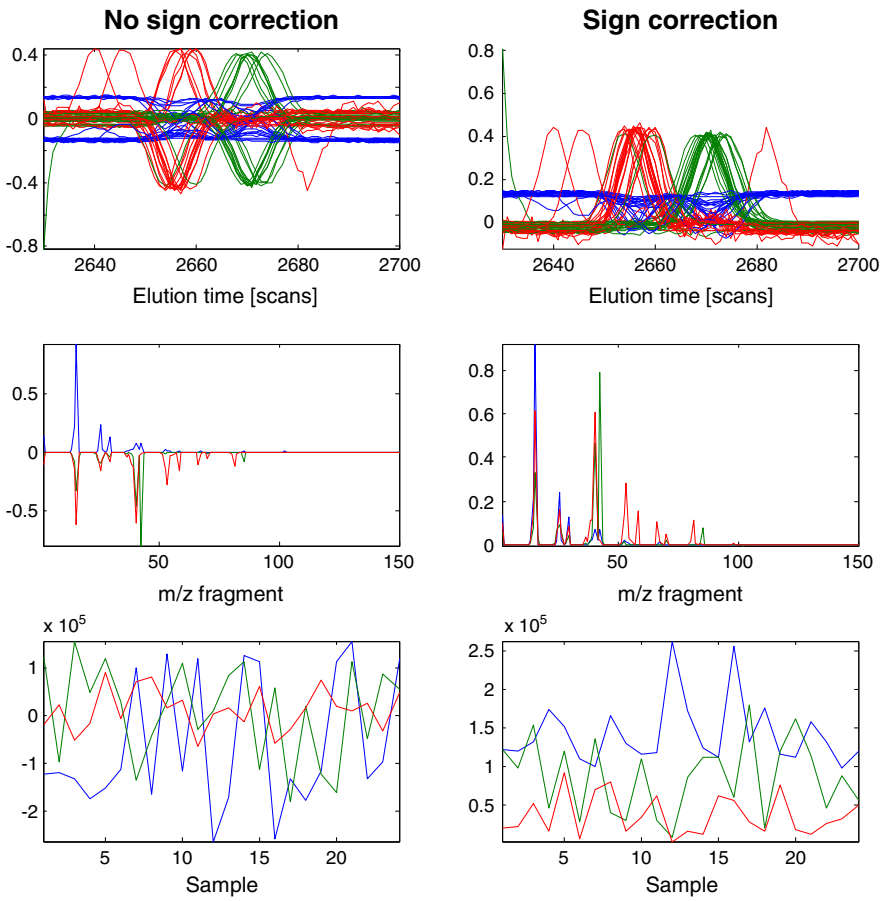

Figure 3. The left side shows the result of a three-component PARAFAC2 model of a chromatographic data set (top: elution mode loadings ($\mathbf{B}_k$); middle: mass spectral loadings (**A**); bottom: sample mode loadings (**C**)). The right side shows the same model upon sign correction.

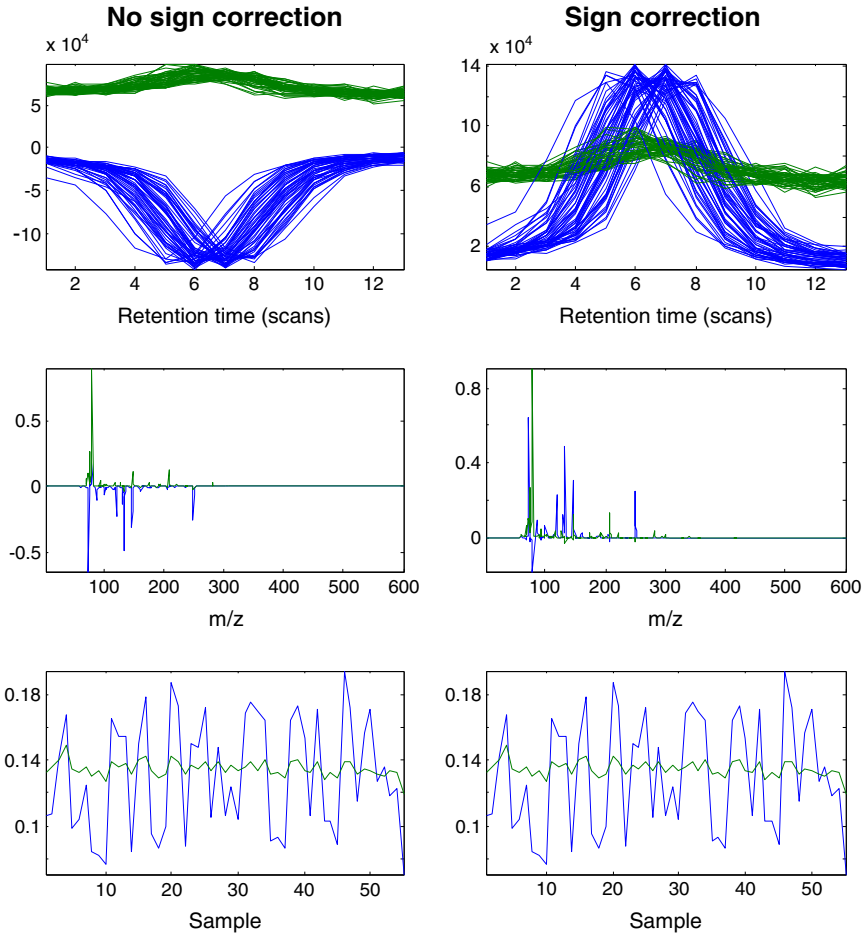

Figure 4. The left side shows the result of a two-factor PARAFAC2 model of a chromatographic data set (top: elution mode loadings; middle: mass spectral loadings; bottom: sample mode loadings). The right side shows the same model upon sign correction. In this example, one of the spectral profiles has been flipped as well as the corresponding elution profiles.

the mass spectral mode, where two loading vectors are exclusively negative. Also note that in the sample mode, the sign indeterminacy means that every element in a given loading vector can change sign independently of others. It is very easy to see in the rightmost sign-corrected version that the sign correction not only is meaningful but also greatly helps in discerning more subtle details of the model.

Another example can be seen in Figure 4. These data come from GC–mass spectrometry analysis of cheese after the samples have been oximated with methoxyamine (20 mg/mL in pyridine) followed by derivatization with N-methyl-N-(trimethylsilyl) trifluoroacetamide (as suggested by Kanani *et al*. [16]). The samples were analyzed on an Agilent Technologies 7890A GC system coupled with a 5975C inert XCMSD detector. In the uncorrected model, it is clear that the loadings for one of the components are turned upside down in the elution time mode as well as in the mass spectral mode. After sign correction, the model appears chemically meaningful with respect to the signs.

3. CONCLUSION

A formal approach has been developed for correcting for sign indeterminacies in various multiway models. Some illustrative examples have been given to show that the correction indeed makes sense from an interpretational point of view.

The sign-correcting function is available at www.models.life.ku.dk (February 2013) as a MATLAB routine.

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