Supplemental material for “Simple enough, but not simpler: reconsidering additive logratio coordinates in compositional analysis”

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A. Derivations of biplot properties

This supplementary material provides detailed derivations of biplot properties discussed in the manuscript in Sections 3.2 and 3.3.

A.1. Compositional case: clr coefficients

- The inner product between the rows of $\mathbf{G}$ and $\mathbf{H}$ (from the decomposition of $\mathbf{Y}$) approximates the clr coefficients:

$$\mathbf{g}_{i\bullet}^T \mathbf{h}_{j\bullet} \approx y_{ij} = \ln \frac{x_{ij}}{g(\mathbf{x}_{i\bullet})}$$

- The length of the rays approximate the variability of clr coefficients corresponding to the parts $\mathbf{x}_j$, $j = 1, \ldots, D$:

$$\|\mathbf{h}_{j\bullet}\|^2 \approx \widehat{\mathrm{var}}(\mathbf{y}_j) = \widehat{\mathrm{var}}\left(\ln \frac{\mathbf{x}_j}{g(\mathbf{x})}\right)$$

- The length of the links between the vertices of the rays approximate the variability of a pairwise logratio formed by the respective parts:

$$\begin{aligned}
\|\mathbf{h}_{i\bullet} - \mathbf{h}_{j\bullet}\|^2 &\approx \frac{1}{n-1}(\mathbf{y}_{\bullet i} - \mathbf{y}_{\bullet j})^T(\mathbf{y}_{\bullet i} - \mathbf{y}_{\bullet j}) = \frac{1}{n-1}\sum_{m=1}^{n}(y_{mi} - y_{mj})^2 = \\
&= \frac{1}{n-1}\sum_{m=1}^{n}\left(\ln \frac{x_{mi}}{g(\mathbf{x}_{m\bullet})} - \frac{x_{mj}}{g(\mathbf{x}_{m\bullet})}\right)^2 = \frac{1}{n-1}\sum_{m=1}^{n}\left(\ln \frac{x_{mi}}{x_{mj}}\right)^2 = \\
&= \widehat{\mathrm{var}}\left(\ln \frac{\mathbf{x}_i}{\mathbf{x}_j}\right)
\end{aligned}$$

- The projection of the i-th score onto a link approximates the difference between the respective clr coefficients (i.e. logratio between x_{ij} and x_{ik}):

$$\mathbf{g}_{i\bullet}^T(\mathbf{h}_{j\bullet} - \mathbf{h}_{k\bullet}) \approx \ln \frac{x_{ij}}{g(\mathbf{x}_{i\bullet})} - \ln \frac{x_{ik}}{g(\mathbf{x}_{i\bullet})} = \ln \frac{x_{ij}}{x_{ik}}$$

A.2. Vector compositional data

- The inner product between a row of the matrix $\mathbf{G}$ and $\mathbf{h}_{1\bullet}^{(l)}$ approximates the pairwise logratio between the l-th component and the rationing part:

$$\mathbf{g}_{i\bullet}^T \mathbf{h}_{1\bullet}^{(l)} = \sqrt{\frac{1}{2}}\left(\mathbf{g}_{i\bullet}^T \mathbf{h}_{l\bullet} - \mathbf{g}_{i\bullet}^T \mathbf{h}_{D\bullet}\right) \approx \sqrt{\frac{1}{2}}(y_{il} - y_{iD}) = \sqrt{\frac{1}{2}} \ln \frac{x_{il}}{x_{iD}}$$

- The lengths of biplot rays approximate the variability of the logratio between the l-th and the rationing part:

$$\|\mathbf{h}_{1\bullet}^{(l)}\|^2 = \sqrt{\frac{1}{2}}(\mathbf{h}_{l\bullet} - \mathbf{h}_{D\bullet})^T \sqrt{\frac{1}{2}}(\mathbf{h}_{l\bullet} - \mathbf{h}_{D\bullet}) = \frac{1}{2}\|\mathbf{h}_{l\bullet} - \mathbf{h}_{D\bullet}\|^2 \approx \frac{1}{2}\widehat{\text{var}}\left(\ln\frac{\mathbf{x}_l}{\mathbf{x}_D}\right)$$

- The length of the links between the vertices of two rays approximate the variability of the logratio between the compositional parts placed in the numerator of the respective pairwise logratios:

$$\|\mathbf{h}_{1\bullet}^{(p)} - \mathbf{h}_{1\bullet}^{(s)}\|^2 = \frac{1}{2}\|(\mathbf{h}_{p\bullet} - \mathbf{h}_{D\bullet}) - (\mathbf{h}_{s\bullet} - \mathbf{h}_{D\bullet})\|^2 = \frac{1}{2}\|\mathbf{h}_{p\bullet} - \mathbf{h}_{s\bullet}\|^2 \approx \frac{1}{2}\widehat{\text{var}}\left(\ln\frac{\mathbf{x}_p}{\mathbf{x}_s}\right)$$

- The projection of a score onto a link approximates the pairwise logratio of the respective components:

$$\mathbf{g}_{i\bullet}^T(\mathbf{h}_{1\bullet}^{(p)} - \mathbf{h}_{1\bullet}^{(s)}) = \mathbf{g}_{i\bullet}^T\mathbf{h}_{1\bullet}^{(p)} - \mathbf{g}_{i\bullet}^T\mathbf{h}_{1\bullet}^{(s)} \approx \sqrt{\frac{1}{2}}\ln\frac{x_{ip}}{x_{iD}} - \sqrt{\frac{1}{2}}\ln\frac{x_{is}}{x_{iD}} = \sqrt{\frac{1}{2}}\ln\frac{x_{ip}}{x_{is}}$$

A.3. Compositional tables

A.3.1. Inter-factorial relations

- The inner product between the rows of the score matrix $\mathbf{G}$ and the first row of $\mathbf{H}^{(kl)}$ approximates the respective simple log odds-ratio:

$$\begin{aligned}
\mathbf{g}_{i\bullet}^T\mathbf{h}_{1\bullet}^{(kl)} &= \frac{1}{2}\left(\mathbf{g}_{i\bullet}^T\mathbf{h}_{[I,J]\bullet} + \mathbf{g}_{i\bullet}^T\mathbf{h}_{[k,l]\bullet} - \mathbf{g}_{i\bullet}^T\mathbf{h}_{[I,l]\bullet} - \mathbf{g}_{i\bullet}^T\mathbf{h}_{[k,J]\bullet}\right) \approx \\
&\approx \frac{1}{2}\left({}_iy_{[I,J]} + {}_iy_{[k,l]} - {}_iy_{[I,l]} - {}_iy_{[k,J]}\right) = \\
&= \frac{1}{2}\left(\ln\frac{{}_ix_{IJ}}{g({}_i\mathbf{x})} + \ln\frac{{}_ix_{kl}}{g({}_i\mathbf{x})} - \ln\frac{{}_ix_{Il}}{g({}_i\mathbf{x})} - \ln\frac{{}_ix_{kJ}}{g({}_i\mathbf{x})}\right) = \frac{1}{2}\ln\frac{{}_ix_{IJ}\,{}_ix_{kl}}{{}_ix_{Il}\,{}_ix_{kJ}}.
\end{aligned}$$

- Due to the centering of the clr coordinate matrix $\mathbf{Y}$ the lengths of the biplot rays approximate the variability of the simple log odds-ratios:

$$\begin{aligned}
\|\mathbf{h}_{1\bullet}^{(kl)}\|^2 &= \frac{1}{4}\|\mathbf{h}_{[I,J]\bullet} + \mathbf{h}_{[k,l]\bullet} - \mathbf{h}_{[I,l]\bullet} - \mathbf{h}_{[k,J]\bullet}\|^2 \approx \\
&\approx \frac{1}{4}\frac{1}{n-1}\|{}_\bullet\mathbf{y}_{[I,J]} + {}_\bullet\mathbf{y}_{[k,l]} - {}_\bullet\mathbf{y}_{[I,l]} - {}_\bullet\mathbf{y}_{[k,J]}\|^2 = \\
&= \frac{1}{4}\frac{1}{n-1}\sum_{m=1}^{n}\left({}_my_{[I,J]} + {}_my_{[k,l]} - {}_my_{[I,l]} - {}_my_{[k,J]}\right)^2 = \\
&= \frac{1}{4}\frac{1}{n-1}\sum_{m=1}^{n}\left(\ln\frac{{}_mx_{IJ}}{g({}_m\mathbf{x})} + \ln\frac{{}_mx_{kl}}{g({}_m\mathbf{x})} - \ln\frac{{}_mx_{Il}}{g({}_m\mathbf{x})} - \ln\frac{{}_mx_{kJ}}{g({}_m\mathbf{x})}\right)^2 = \\
&= \frac{1}{4}\frac{1}{n-1}\sum_{m=1}^{n}\left(\ln\frac{{}_mx_{IJ}\,{}_mx_{kl}}{{}_mx_{Il}\,{}_mx_{kJ}}\right)^2 = \frac{1}{4}\widehat{\text{var}}\left(\ln\frac{x_{IJ}x_{kl}}{x_{Il}x_{kJ}}\right).
\end{aligned}$$

- The length of the links between two vertices can in general be understood in terms of difference between variation of the respective simple log odds-ratios. Moreover, a more convenient interpretation is available for some combinations. Thus, the links between rays related to odds-ratios sharing two common elements approximate the variation of a new simple log odds-ratio. Considering e.g. the log odds-ratios sharing the elements at positions $[k,J]$ and $[I,J]$, and differing in the column permutation index l (represented by $\mathbf{h}_{1\bullet}^{(kl_1)}$ and $\mathbf{h}_{1\bullet}^{(kl_2)}$, $l_1 \neq l_2$), the distance between the corresponding rays verifies that

$$\begin{aligned}\|\mathbf{h}_{1\bullet}^{(kl_1)} - \mathbf{h}_{1\bullet}^{(kl_2)}\|^2 &= \frac{1}{4}\|\left(\mathbf{h}_{[I,J]\bullet} + \mathbf{h}_{[k,l_1]\bullet} - \mathbf{h}_{[I,l_1]\bullet} - \mathbf{h}_{[k,J]\bullet}\right) - \\ &\quad - \left(\mathbf{h}_{[I,J]\bullet} + \mathbf{h}_{[k,l_2]\bullet} - \mathbf{h}_{[I,l_2]\bullet} - \mathbf{h}_{[k,J]\bullet}\right)\|^2 = \\ &= \frac{1}{4}\|\mathbf{h}_{[k,l_1]\bullet} - \mathbf{h}_{[I,l_1]\bullet} - \mathbf{h}_{[k,l_2]\bullet} + \mathbf{h}_{[I,l_2]\bullet}\|^2 \approx \\ &\approx \frac{1}{4}\frac{1}{n-1}\|{}_{\bullet}\mathbf{y}_{[k,l_1]} + {}_{\bullet}\mathbf{y}_{[I,l_2]} - {}_{\bullet}\mathbf{y}_{[I,l_1]} - {}_{\bullet}\mathbf{y}_{[k,l_2]}\|^2 = \\ &= \frac{1}{4}\frac{1}{n-1}\sum_{m=1}^{n}\left(\ln\frac{{}_{m}x_{kl_1}\,{}_{m}x_{Il_2}}{{}_{m}x_{Il_1}\,{}_{m}x_{kl_2}}\right)^2 = \frac{1}{4}\widehat{\mathrm{var}}\left(\ln\frac{x_{kl_1}x_{Il_2}}{x_{Il_1}x_{kl_2}}\right),\end{aligned}$$

  with ${}_{\bullet}\mathbf{y}_{[i,j]}$ representing the vector of all clr coefficients $\mathbf{y}_{[i,j]}$ from the sample.

  A similar derivation can be given for odds-ratios sharing the same column indices, i.e. $x_{k_1l}x_{IJ}/x_{k_1J}x_{Il}$ and $x_{k_2l}x_{IJ}/x_{k_2J}x_{Il}$ for $k_1 \neq k_2$, where the corresponding link estimates the variance of $\ln\left(x_{k_1l}x_{k_2J}/x_{k_1J}x_{k_2l}\right)$. Consequently, when a biplot collects results from all coordinate systems defined for a fixed rationing part x_{IJ}, it preserves also the information on the variability of the odds-ratios containing parts either from the I-th row or the J-th column. On the other hand, the characteristics of the other odds-ratios are not represented in this setting.

- In the case of the projection of a score to a link, only pairs of odds-ratios sharing elements from the same row or column are worth investigating. E.g. for the same pair as considered in the previous point, it holds that

$$\begin{aligned}\mathbf{g}_{i\bullet}^T(\mathbf{h}_{1\bullet}^{(kl_1)} - \mathbf{h}_{1\bullet}^{(kl_2)}) &= \mathbf{g}_{i\bullet}^T\left[\frac{1}{2}\left(\mathbf{h}_{[I,J]\bullet} + \mathbf{h}_{[k,l_1]\bullet} - \mathbf{h}_{[I,l_1]\bullet} - \mathbf{h}_{[k,J]\bullet}\right) - \right. \\ &\quad \left. - \frac{1}{2}\left(\mathbf{h}_{[I,J]\bullet} + \mathbf{h}_{[k,l_2]\bullet} - \mathbf{h}_{[I,l_2]\bullet} - \mathbf{h}_{[k,J]\bullet}\right)\right] = \\ &= \frac{1}{2}\left(\mathbf{g}_{i\bullet}^T\mathbf{h}_{[k,l_1]\bullet} - \mathbf{g}_{i\bullet}^T\mathbf{h}_{[I,l_1]\bullet} - \mathbf{g}_{i\bullet}^T\mathbf{h}_{[k,l_2]\bullet} + \mathbf{g}_{i\bullet}^T\mathbf{h}_{[I,l_2]\bullet}\right) \approx \\ &\approx \frac{1}{2}\left({}_{i}y_{[k,l_1]} + {}_{i}y_{[I,l_2]} - {}_{i}y_{[I,l_1]} - {}_{i}y_{[k,l_2]}\right) = \\ &= \frac{1}{2}\left(\ln\frac{{}_{i}x_{kl_1}}{g({}_{i}\mathbf{x})} + \ln\frac{{}_{i}x_{Il_2}}{g({}_{i}\mathbf{x})} - \ln\frac{{}_{i}x_{Il_1}}{g({}_{i}\mathbf{x})} - \ln\frac{{}_{i}x_{kl_2}}{g({}_{i}\mathbf{x})}\right) = \frac{1}{2}\ln\frac{{}_{i}x_{kl_1}\,{}_{i}x_{Il_2}}{{}_{i}x_{Il_1}\,{}_{i}x_{kl_2}}.\end{aligned}$$

A.3.2. Intra-factorial relations

- The inner product between a row of matrix $\mathbf{G}$ and $\mathbf{h}_{r1\bullet}^{(kl)}$ approximates the pairwise row balance:

$$\mathbf{g}_{i\bullet}^T\mathbf{h}_{r1\bullet}^{(kl)} = \sqrt{\frac{1}{2J}}\left(\mathbf{g}_{i\bullet}^T\mathbf{h}_{[k,1]\bullet} + \ldots + \mathbf{g}_{i\bullet}^T\mathbf{h}_{[k,J]\bullet} - \mathbf{g}_{i\bullet}^T\mathbf{h}_{[I,1]\bullet} - \ldots - \mathbf{g}_{i\bullet}^T\mathbf{h}_{[I,J]\bullet}\right) \approx$$
$$\approx \sqrt{\frac{1}{2J}}\left({}_iy_{[k,1]} + \ldots + {}_iy_{[k,J]} - {}_iy_{[I,1]} - \ldots - {}_iy_{[I,J]}\right) = \sqrt{\frac{J}{2}}\ln\frac{g\left({}_i\mathbf{x}_{k\bullet}\right)}{g\left({}_i\mathbf{x}_{I\bullet}\right)}.$$

- The lengths of the biplot rays give an approximation of the variability of the pairwise row balances:

$$\|\mathbf{h}_{r1\bullet}^{(kl)}\|^2 = \frac{1}{2J}\|\mathbf{h}_{[k,1]\bullet} + \ldots + \mathbf{h}_{[k,J]\bullet} - \mathbf{h}_{[I,1]\bullet} - \ldots - \mathbf{h}_{[I,J]\bullet}\|^2 \approx$$
$$\approx \frac{1}{2J}\frac{1}{n-1}\|{}_\bullet\mathbf{y}_{[k,1]} + \ldots + {}_\bullet\mathbf{y}_{[k,J]} - {}_\bullet\mathbf{y}_{[I,1]} - \ldots - {}_\bullet\mathbf{y}_{[I,J]}\|^2 =$$
$$= \frac{1}{2J}\frac{1}{n-1}\sum_{m=1}^{n}\left({}_my_{[k,1]} + \ldots + {}_my_{[k,J]} - {}_my_{[I,1]} - \ldots - {}_my_{[I,J]}\right)^2 =$$
$$= \frac{J}{2}\widehat{\text{var}}\left(\ln\frac{g(\mathbf{x}_{k\bullet})}{g(\mathbf{x}_{I\bullet})}\right).$$

- The length of the links between the vertices of the rays approximate the variability of the balance between row categories standing in the numerator of the respective coordinates:

$$\|\mathbf{h}_{r1\bullet}^{(k_1l)} - \mathbf{h}_{r1\bullet}^{(k_2l)}\|^2 = \frac{1}{2J}\|\left(\mathbf{h}_{[k_1,1]\bullet} + \ldots + \mathbf{h}_{[k_1,J]\bullet} - \mathbf{h}_{[I,1]\bullet} - \ldots - \mathbf{h}_{[I,J]\bullet}\right) -$$
$$- \left(\mathbf{h}_{[k_2,1]\bullet} + \ldots + \mathbf{h}_{[k_2,J]\bullet} - \mathbf{h}_{[I,1]\bullet} - \ldots - \mathbf{h}_{[I,J]\bullet}\right)\|^2 \approx$$
$$\approx \frac{1}{2J}\frac{1}{n-1}\|{}_\bullet\mathbf{y}_{[k_1,1]} + \ldots + {}_\bullet\mathbf{y}_{[k_1,J]} - {}_\bullet\mathbf{y}_{[k_2,1]} - \ldots - {}_\bullet\mathbf{y}_{[k_2,J]}\|^2 =$$
$$= \frac{J}{2}\widehat{\text{var}}\left(\ln\frac{g(\mathbf{x}_{k_1\bullet})}{g(\mathbf{x}_{k_2\bullet})}\right).$$

- A specific pairwise row balance can be for a given observation approximated by the projection to a link:

$$\mathbf{g}_{i\bullet}^T\left(\mathbf{h}_{r1\bullet}^{(k_1l)} - \mathbf{h}_{r1\bullet}^{(k_2l)}\right) = \mathbf{g}_{i\bullet}^T\mathbf{h}_{r1\bullet}^{(k_1l)} - \mathbf{g}_{i\bullet}^T\mathbf{h}_{r1\bullet}^{(k_2l)} \approx$$
$$\approx \sqrt{\frac{J}{2}}\ln\frac{g\left({}_i\mathbf{x}_{k_1\bullet}\right)}{g\left({}_i\mathbf{x}_{I\bullet}\right)} - \sqrt{\frac{J}{2}}\ln\frac{g\left({}_i\mathbf{x}_{k_2\bullet}\right)}{g\left({}_i\mathbf{x}_{I\bullet}\right)} = \sqrt{\frac{J}{2}}\ln\frac{g\left({}_i\mathbf{x}_{k_1\bullet}\right)}{g\left({}_i\mathbf{x}_{k_2\bullet}\right)}.$$

B. Construction of backwards pivot coordinates

This supplementary material serves as a thorough guide for construction of backwards pivot coordinates to represent both vector compositional data and compositional tables, which is discussed in Sections 2.1 and 2.2 of the manuscript. The following two sections refer to compositional vector case and compositional tables case respectively.

B.1. Compositional vectors

Considering a D-part composition with a rationing part x_D and a (pivot) part x_l, this composition can be rearranged into a permuted one $\mathbf{x}^{(l)}$ with rationing part in the first position and x_l in the second position, followed by construction of backwards pivot coordinate system. The procedure is illustrated in the following scheme:

$$\mathbf{x} = (x_1, x_2, \dots, x_{l-1}, \boxed{x_l}, x_{l+1}, \dots, x_{D-1}, \boxed{x_D})$$

$$\Downarrow$$

$$\begin{aligned} \mathbf{x}^{(l)} &= (\boxed{x_D}, \boxed{x_l}, x_1, x_2, \dots, x_{l-1}, x_{l+1}, \dots, x_{D-1}) \\ &= (\boxed{x_1^{(l)}}, \boxed{x_2^{(l)}}, x_3^{(l)}, x_4^{(l)}, \dots, x_{l+1}^{(l)}, x_{l+2}^{(l)}, \dots, x_D^{(l)}) \end{aligned}$$

$$\Downarrow$$

i	x_D $x_1^{(l)}$	x_l $x_2^{(l)}$	x_1 $x_3^{(l)}$	x_2 $x_4^{(l)}$	$\cdots$ $\cdots$	x_{D-1} $x_D^{(l)}$
1	$-$	$+$	0	0	$\cdots$	0
2	$-$	$-$	$+$	0	$\cdots$	0
3	$-$	$-$	$-$	$+$	$\cdots$	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$D-1$	$-$	$-$	$-$	$-$	$\cdots$	$+$

Table S.1. *SBP for compositional vector case.*

The first backwards pivot coordinate is then given by equation (S1).

$$\mathrm{bpc}(\mathbf{x}^{(l)})_1 = \frac{1}{\sqrt{2}} \ln \frac{\boxed{x_2^{(l)}}}{\boxed{x_1^{(l)}}} = \frac{1}{\sqrt{2}} \ln \frac{\boxed{x_l}}{\boxed{x_D}}. \tag{S1}$$

B.2. Compositional tables

Let $\mathbf{x}$ denote a compositional table consisting of I rows and J columns and assume that $\mathbf{x}^{(kl)}$ is its permutation. In this case, the normalizing parts are I-th row and J-column (being placed to the first position; colored in light yellow in the visualisation), leading to a part x_{IJ} being in the position $[1,1]$ in $\mathbf{x}^{(kl)}$ and having the same role as x_D in the vector case. Moreover, k-th row and l-th column are placed in the second position (colored in light blue in the visualisation), resulting in a part x_{kl} in the position $[2,2]$ in the permuted table and playing the role of the pivoting part (x_l in the vector case). Parts highlighted in intense colors will be further used for construction of table backwards pivot coordinates. The original compositional table $\mathbf{x}$ with highlighted normalizing and pivoting rows and columns is shown in Figure S.1, while the permuted table is $\mathbf{x}^{(kl)}$ is given in Figure S.2.

$$\mathbf{x} = \begin{array}{c c}
\begin{array}{ccccccccc} \phantom{x_{k-11}} & \phantom{x_{k-12}} & & \phantom{x_{k-1l-1}} & \mathbf{x_{\bullet l}} & \phantom{x_{k-1l+1}} & & \phantom{x_{k-1J-1}} & \mathbf{x_{\bullet J}} \end{array} & \\
\begin{pmatrix}
x_{11} & x_{12} & \cdots & x_{1l-1} & x_{1l} & x_{1l+1} & \cdots & x_{1J-1} & x_{1J} \\
x_{21} & x_{22} & \cdots & x_{2l-1} & x_{2l} & x_{2l+1} & \cdots & x_{2J-1} & x_{2J} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
x_{k-11} & x_{k-12} & \cdots & x_{k-1l-1} & x_{k-1l} & x_{k-1l+1} & \cdots & x_{k-1J-1} & x_{k-1J} \\
x_{k1} & x_{k2} & \cdots & x_{kl-1} & x_{kl} & x_{kl+1} & \cdots & x_{kJ-1} & x_{kJ} \\
x_{k+11} & x_{k+12} & \cdots & x_{k+1l-1} & x_{k+1l} & x_{k+1l+1} & \cdots & x_{k+1J-1} & x_{k+1J} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
x_{I-11} & x_{I-12} & \cdots & x_{I-1l-1} & x_{I-1l} & x_{I-1l+1} & \cdots & x_{I-1J-1} & x_{I-1J} \\
x_{I1} & x_{I2} & \cdots & x_{Il-1} & x_{Il} & x_{Il+1} & \cdots & x_{IJ-1} & x_{IJ}
\end{pmatrix} &
\begin{array}{c} \\ \\ \\ \\ \mathbf{x_{k\bullet}} \\ \\ \\ \\ \mathbf{x_{I\bullet}} \end{array}
\end{array}$$

Figure S.1. *Compositional table with highlighted normalizing (light yellow color) and pivoting (light blue color) rows and columns. Parts colored in intense colors appear in table backwards pivot coordinates.*

$$\mathbf{x}^{(kl)} = \begin{array}{c c}
\begin{array}{ccccccccc} \mathbf{x^{(kl)}_{\bullet 1}} & \mathbf{x^{(kl)}_{\bullet 2}} & \phantom{x_{k-11}} & \phantom{x_{k-12}} & & \phantom{x_{k-1l-1}} & \phantom{x_{k-1l+1}} & & \phantom{x_{k-1J-1}} \end{array} & \\
\begin{pmatrix}
x_{IJ} & x_{Il} & x_{I1} & x_{I2} & \cdots & x_{Il-1} & x_{Il+1} & \cdots & x_{IJ-1} \\
x_{kJ} & x_{kl} & x_{k1} & x_{k2} & \cdots & x_{kl-1} & x_{kl+1} & \cdots & x_{kJ-1} \\
x_{1J} & x_{1l} & x_{11} & x_{12} & \cdots & x_{1l-1} & x_{1l+1} & \cdots & x_{1J-1} \\
x_{2J} & x_{2l} & x_{21} & x_{22} & \cdots & x_{2l-1} & x_{2l+1} & \cdots & x_{2J-1} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
x_{k-1J} & x_{k-1l} & x_{k-11} & x_{k-12} & \cdots & x_{k-1l-1} & x_{k-1l+1} & \cdots & x_{k-1J-1} \\
x_{k+1J} & x_{k+1l} & x_{k+11} & x_{k+12} & \cdots & x_{k+1l-1} & x_{k+1l+1} & \cdots & x_{k+1J-1} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
x_{I-1J} & x_{I-1l} & x_{I-11} & x_{I-12} & \cdots & x_{I-1l-1} & x_{I-1l+1} & \cdots & x_{I-1J-1}
\end{pmatrix} &
\begin{array}{c} \mathbf{x^{(kl)}_{1\bullet}} \\ \mathbf{x^{(kl)}_{2\bullet}} \\ \\ \\ \\ \\ \\ \\ \\ \end{array}
\end{array} = (x_{ij}^{(kl)})$$

Figure S.2. *Permutation of the original compositional table.*

Table S.2 demonstrates SBP partitions for row balances (SBPr) and column balances (SBPc), respectively.

Following the aforementioned steps, the first pairwise row balance is given by equation (S2) and a simple corresponding chart is shown in Table S.3.

i	x_I $x_{1\bullet}^{(k)}$	x_k $x_{2\bullet}^{(k)}$	x_1 $x_{3\bullet}^{(k)}$	x_2 $x_{4\bullet}^{(k)}$	$\cdots$ $\cdots$	x_{I-2} $x_{I-1\bullet}^{(k)}$	x_{I-1} $x_{I\bullet}^{(k)}$
1	$-$	$+$	0	0	$\cdots$	$-$	0
2	$-$	$-$	$+$	0	$\cdots$	$-$	0
3	$-$	$-$	$-$	$+$	$\cdots$	$-$	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$I-2$	$-$	$-$	$-$	$-$	$\cdots$	$+$	0
$I-1$	$-$	$-$	$-$	$-$	$\cdots$	$-$	$+$

j	x_J $x_{\bullet 1}^{(l)}$	x_l $x_{\bullet 2}^{(l)}$	x_1 $x_{\bullet 3}^{(l)}$	x_2 $x_{\bullet 4}^{(l)}$	$\cdots$ $\cdots$	x_{J-2} $x_{\bullet J-1}^{(l)}$	x_{J-1} $x_{\bullet J}^{(l)}$
1	$-$	$+$	0	0	$\cdots$	$-$	0
2	$-$	$-$	$+$	0	$\cdots$	$-$	0
3	$-$	$-$	$-$	$+$	$\cdots$	$-$	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$J-2$	$-$	$-$	$-$	$-$	$\cdots$	$+$	0
$J-1$	$-$	$-$	$-$	$-$	$\cdots$	$-$	$+$

Table S.2. *SBPr (upper panel) and SBPc (lower panel).*

$$\mathrm{rbpb}(\mathbf{x}^{(kl)})_1 = \sqrt{\frac{J}{2}} \ln \frac{g(\mathbf{x}_{2\bullet}^{(kl)})}{g(\mathbf{x}_{1\bullet}^{(kl)})} = \sqrt{\frac{J}{2}} \ln \frac{g(\mathbf{x}_{k\bullet})}{g(\mathbf{x}_{I\bullet})} \tag{S2}$$

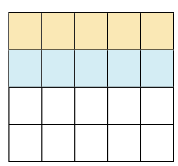

Table S.3. *Visual representation of the rows constituting the first row backwards pivot balance, based on the permuted table* $\mathbf{x}^{(kl)}$.

The first pairwise column balance is constructed analogously. It can be formally written as in equation (S3), followed by the chart in Table S.4.

$$\mathrm{cbpb}(\mathbf{x}^{(kl)})_1 = \sqrt{\frac{I}{2}} \ln \frac{g(\mathbf{x}_{\bullet 2}^{(kl)})}{g(\mathbf{x}_{\bullet 1}^{(kl)})} = \sqrt{\frac{I}{2}} \ln \frac{g(\mathbf{x}_{\bullet l})}{g(\mathbf{x}_{\bullet J})} \tag{S3}$$

Finally, the first table backwards pivot coordinate, which reflects the relation between the factors, is given by equation (S4) and visually shown in the Table S.5.

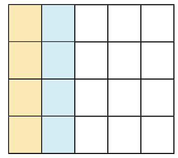

Table S.4. *Visual representation of the columns constituting the first column backwards pivot balance, based on the permuted table* $\mathbf{x}^{(kl)}$.

$$\mathrm{tbpc}(\mathbf{x}^{(kl)})_{11} = \frac{1}{2}\ln\frac{x_{11}^{(kl)}x_{22}^{(kl)}}{x_{12}^{(kl)}x_{21}^{(kl)}} = \frac{1}{2}\ln\frac{x_{IJ}\,x_{kl}}{x_{Il}x_{kJ}}. \tag{S4}$$

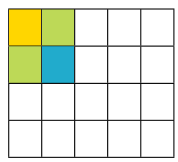

Table S.5. *Visual representation of parts constituting the first table backwards pivot coordinate, based on the permuted table* $\mathbf{x}^{(kl)}$.