# Supplemental material for "Subcompositional coherence and a novel proportionality index of parts"

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## A. Aitchison geometry for compositional data

Aitchison geometry is here referred to $K$-part compositions, where $K$ can take different values like $D$, $d$, $N$ or $n$ when dealing with $(N,D)$ data matrices or their respective subcompositions and subsamples as used in Appendix B. For a $K$-part compositions $\mathbf{x} = (x_1, x_2, \ldots, x_K)^\top$, $\mathbf{y} = (y_1, y_2, \ldots, y_K)^\top$, $\alpha \in \mathbb{R}$, $\mathcal{C}$ denoting closure and $(^\top)$ denoting transposition, the operations and metrics defined in the $K$-part simplex, $\mathbb{S}^K$, are the following:

**Definition A.1** (Euclidean space operations and metrics)**.**

$$\text{Perturbation:} \qquad \mathbf{x} \oplus \mathbf{y} = \mathcal{C}\left(x_1 \cdot y_1, x_2 \cdot y_2, \ldots, x_K \cdot y_K\right)^\top .$$

$$\text{Powering by a scalar:} \qquad \alpha \odot \mathbf{x} = \mathcal{C}\left(\alpha \odot \mathbf{x}\right) = \mathcal{C}\left(x_1^\alpha, x_2^\alpha, \ldots, x_K^\alpha\right)^\top .$$

$$\text{Inner product:} \qquad \langle \mathbf{x}, \mathbf{y} \rangle_a = \frac{1}{2K} \sum_{i=1}^{K} \sum_{j=1}^{K} \ln \frac{x_i}{x_j} \ln \frac{y_i}{y_j} .$$

**Definition A.2** (Aitchison norm and distance)**.**

$$\|\mathbf{x}\|_a = \langle \mathbf{x}, \mathbf{x} \rangle_a , \quad \mathrm{d}_a\left(\mathbf{x}, \mathbf{y}\right) = \|\mathbf{x} \ominus \mathbf{y}\|_a .$$

The centred log-ratio transformation (clr) plays an important role in the Aitchison geometry although it does not provide minimal log-ratio coordinates representing compositions.

**Definition A.3** (centred log-ratio transformation)**.** Let $\mathbf{x} = (x_1, x_2, \ldots, x_K)^\top$ be a $K$-part composition, not necessarily represented in $\mathbb{S}^K$. Its centred log-ratio transformation (clr) is

$$\mathrm{clr}(\mathbf{x}) = \left(\log \frac{x_1}{\mathrm{g_m}(\mathbf{x})}, \log \frac{x_2}{\mathrm{g_m}(\mathbf{x})}, \ldots, \log \frac{x_K}{\mathrm{g_m}(\mathbf{x})}\right)^\top ,$$

where $\mathrm{g_m}(\cdot)$ is the geometric mean of the arguments.

The fact that the sum of all components of $\mathrm{clr}(\mathbf{x})$ is null is remarkable. The expression of the Aitchison inner product is simplified using clr since $\langle \mathbf{x}, \mathbf{y} \rangle_a = \langle \mathrm{clr}(\mathbf{x}), \mathrm{clr}(\mathbf{y}) \rangle_e$, where $\langle \cdot, \cdot \rangle_e$ is the ordinary inner product in $\mathbb{R}^K$.

The assignation of orthogonal Cartesian coordinates to a composition is called isometric log-ratio transformation (ilr) (Egozcue et al., 2003; Pawlowsky-Glahn et al., 2015) and is defined as follows.

**Definition A.4** (isometric log-ratio coordinates)**.** The ilr coordinates of a $K$-part composition $\mathbf{x}$ are

$$\mathbf{z} = \mathrm{ilr}(\mathbf{x}) = V^\top \mathrm{clr}(\mathbf{x}) \quad , \quad V^\top V = \mathrm{I}_{K-1} ,$$

where $V$ is a $K \times (K-1)$ matrix, called contrast matrix, and $\mathrm{I}_{K-1}$ the identity matrix of order $K-1$.

Linear functions, from the simplex $\mathbb{S}^K$ onto $\mathbb{R}$, are identified to the scale invariant log-contrasts

$$\phi(\mathbf{x}) = \sum_{i=1}^{K} \alpha_i \log x_i \quad , \quad \sum_{i=1}^{K} \alpha_i = 0 \ ,$$

where the last condition on the coefficients $\alpha_i$ assures that $\phi$ is scale invariant (Aitchison, 1986; Egozcue and Pawlowsky-Glahn, 2019). Special cases of log-contrasts, called *balances*, were introduced in Egozcue and Pawlowsky-Glahn (2005). A balance between two non-overlapping groups of parts, $G$, $H$, has the form

$$B(G/H) = \sqrt{\frac{n_G n_H}{n_G + n_H}} \log \frac{\mathrm{g_m}(G)}{\mathrm{g_m}(H)} \ ,$$

where $\mathrm{g_m}(G)$, and $\mathrm{g_m}(H)$ are the geometric means of the parts included in the groups $G$ and $H$ respectively. Balances are simple since the $\alpha_i$'s of their log-contrasts only attain one of three different values, namely a positive value, a negative value, or zero. Furthermore, they can be sparse if the involved groups of parts $G$ and $H$ do contain only a few parts of $\mathbf{x}$.

A particular case of ilr-coordinates in which each coordinate is a balance can be obtained by a sequential binary partition (SBP) of the parts of the composition as explained in Egozcue and Pawlowsky-Glahn (2006) or Pawlowsky-Glahn et al. (2015).

## B. Relations between spaces of parts and observations.

### *B.1. Compositional samples*

When $\mathbf{X}$ is viewed as a matrix of observed ($o$) compositions, statistical elements show up as important. Between them, $o$-centre, $o$-variation matrix, $o$-total variance, and $o$-Aitchison interdistances play an important role in compositional exploratory analysis. Similarly, $\mathbf{X}^\top$ can be considered as a compositional sample and the original parts ($p$) appear as compositions. Then $p$ versions of the mentioned statistics can be also considered (Pawlowsky-Glahn and Egozcue, 2022).

In order to discuss these points, consider a compositional sample in a matrix $\mathbf{X}$, whose rows are observed compositions $\mathbf{x}_i$, $i = 1, 2, \ldots, N$, and $X_j$, $j = 1, 2, \ldots, D$ are the $D$-columns that are named *parts*. Then,

$$\mathbf{X} = (X_1, X_2, \ldots, X_D) = (\mathbf{x}_1^\top, \mathbf{x}_2^\top, \ldots, \mathbf{x}_N^\top)^\top \ .$$

An elementary statistical concept is that of sample centre, the compositional counterpart of the average or sample mean in real variables.

**Definition B.1.** (Sample centre of observations and parts) The sample centre of $\mathbf{X}$ in $\mathcal{O}^D$ and $\mathcal{P}^N$ are, respectively,

$$\mathrm{Cen}_o(\mathbf{X}) = \left(\frac{1}{N}\right) \odot_o \bigoplus_{o,i=1}^{N} \mathbf{x}_i \quad , \quad \mathrm{Cen}_p(\mathbf{X}) = \left(\frac{1}{D}\right) \odot_p \bigoplus_{p,j=1}^{D} X_j \ . \tag{B.1}$$

When considering $\mathcal{C}_o(\mathbf{X})$ ($\mathcal{C}_p(\mathbf{X})$) the sample centre $\mathrm{Cen}_o(\mathbf{X})$ ($\mathrm{Cen}_p(\mathbf{X})$) can be identified with the closed vector of geometric means by columns (rows).

The sample matrix $\mathbf{X}$ can be closed to 1 by rows dividing the entries $\mathbf{x}_i$ by the sum of all its elements by rows, $S_i = \sum_{j=1}^{D} x_{ij}$. The matrix whose rows are $\mathcal{C}\mathbf{x}_i$ is denoted $\mathcal{C}_o\mathbf{X}$. Let $\mathcal{C}_o\mathbf{Y}$ denote the $(N,d)$-matrix with entries $y_{ij} = x_{ij}/s_i$, where $s_i = \sum_{j=1}^{d} x_{ij}$, so that the rows of $\mathcal{C}_o\mathbf{Y}$, are closed to 1. Therefore, $\mathcal{C}_o\mathbf{Y}$ is the sample after taking a subcomposition followed by closure by rows. Similarly, the parts (columns) of $\mathbf{X}$ can be closed by dividing the $X_j$ part by $\sum_{i=1}^{N} x_{ij}$. If necessary the data matrix with closed parts is denoted by $\mathcal{C}_p\mathbf{X}$. Observations $\mathbf{x}_i$ are compositions represented in $\mathcal{O}^D \equiv \mathbb{S}^D$ and the parts are in $\mathcal{P}^N \equiv \mathbb{S}^N$.

Some properties are now straightforward to derive, most of them reported in Pawlowsky-Glahn and Egozcue (2022).

**Proposition B.1.** *Closure of observations $\mathbf{x}_i$ in $\mathbf{X}$ is a p-perturbation in $\mathcal{P}^N$, while closure of parts $X_j$ in $\mathbf{X}$ is an o-perturbation in $\mathcal{O}^D$.*

*Proof.* The closure of observations (Definition 2.2), i.e. rows $\mathbf{x}_i$ of $\mathbf{X}$, consists in computing first the sum $s_{oi} = \sum_{j=1}^{D} x_{ij}$ of each row, and then multiplying each part in one row by $s_{oi}^{-1}$. Denoting the perturbation-subtraction by $\ominus_p$ and $\mathbf{s}_o = (s_{o1}, s_{o2}, \ldots, s_{oN})^\top$, this can be written as

$$\mathcal{C}_o(\mathbf{X}) = (X_1 \ominus_p \mathbf{s}_o, X_2 \ominus_p \mathbf{s}_o, \ldots, X_D \ominus_p \mathbf{s}_o) \ ,$$

which is a $p$-perturbation. Analogous reasoning holds to proof that

$$\mathcal{C}_p(\mathbf{X}) = \left( (\mathbf{x}_1 \ominus_o \mathbf{s}_p)^\top, (\mathbf{x}_2 \ominus_o \mathbf{s}_p)^\top, \ldots, (\mathbf{x}_N \ominus_o \mathbf{s}_p)^\top \right)^\top$$

with $\mathbf{s}_p = (s_{p1}, s_{p2}, \ldots, s_{pD})^\top$ and $s_{pj} = \sum_{i=1}^{N} x_{ij}$. ■

A consequence of Proposition B.1 is that taking a $d$-subcomposition of rows in $\mathbf{X}$, followed by the closure of each row, implies a $p$-perturbation of parts on the $d$-remaining parts. Similarly, taking a subsample of $\mathbf{X}$, that is removing $N-n$ rows and maintaining $n$ observations, conventionally, the first $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$, and then closing them, induces an $o$-perturbation in the remaining columns.

Also, column (row) operations, like centring or perturbation average, that imply a previous closure to proceed, induce an $o$-perturbation ($p$-perturbation) on the rows (columns).

**Definition B.2** (Variation matrix)**.** Let $\mathbf{X}$ be an $(N \times D)$-compositional data matrix. The $o$-variation and $p$-variation matrices are, respectively, $(D \times D)$ and $(N \times N)$ matrices $T^o$ and $T^p$, with entries

$$t_{kj}^{o} = \mathrm{Var}_p \left[ \log \frac{X_k}{X_j} \right] \ , \quad t_{ki}^{p} = \mathrm{Var}_o \left[ \log \frac{\mathbf{x}_k}{\mathbf{x}_i} \right] \ ,$$

where $\mathrm{Var}_p$ is the sample variance taken along $p$-columns and $\mathrm{Var}_o$ is the sample variance taken along $o$-rows.

**Definition B.3.** (Total variance) The total variance of observations and parts are

$$\mathrm{totVar}_o(\mathbf{X}) = \frac{1}{2D} \sum_{k=1}^{D} \sum_{j=1}^{D} t^o_{kj} \ , \quad \mathrm{totVar}_p(\mathbf{X}) = \frac{1}{2N} \sum_{i=1}^{N} \sum_{k=1}^{N} t^p_{ki} \ ,$$

respectively.

This definition of total variance was given in Aitchison (1986). However, it can be defined in several ways that help to understand the different log-ratio representations of compositions.

As shown in Egozcue and Pawlowsky-Glahn (2011),

$$\mathrm{totVar}_o(\mathbf{X}) = \sum_{j=1}^{D} \mathrm{Var}_p(\mathrm{clr}_j(\mathbf{x})) = \sum_{k=1}^{D-1} \mathrm{Var}_p(\mathrm{ilr}_k(\mathbf{x})) \ , \tag{B.2}$$

$$\mathrm{totVar}_p(\mathbf{X}) = \sum_{i=1}^{N} \mathrm{Var}_o(\mathrm{clr}_i(X)) = \sum_{k=1}^{N-1} \mathrm{Var}_o(\mathrm{ilr}_k(X)) \ , \tag{B.3}$$

### *B.2. Subcompositions in a sample*

The question is how we can identify $\mathcal{C}_o\mathbf{Y}$ as a subcompositional sample of $\mathcal{C}_o\mathbf{X}$. To give an answer to this question, consider that columns of both $\mathbf{X}$ and $\mathbf{Y}$ are also compositions, in general not closed. The matrix $\mathcal{C}_o\mathbf{Y}$ has columns $Y_1, Y_2, \dots, Y_d$ and they are perturbative shifts of $X_1, X_2, \dots, X_d$ in $\mathbf{X}$, that is $Y_j = X_j \oplus p_j$ for $j = 1, 2, \dots, d$ and some perturbation $\mathbf{p} = (p_1, p_2, \dots, p_N)^\top$ which depends on the parts excluded from the subcomposition $X_{d+1}, X_{d+2}, \dots, X_D$.

The dominance of the Aitchison distance under a subcomposition is well-known (Aitchison, 1992). For observations and parts, dominance can be formulated as

**Proposition B.2.** *For any subcomposition* $\mathbf{Y}$ *of* $\mathbf{X}$ *containing the observations* $\mathbf{x}_1$, $\mathbf{x}_2$*, it holds*

$$\mathrm{d}_o(\mathbf{x}_1, \mathbf{x}_2) \geq \mathrm{d}_o(\mathbf{y}_1, \mathbf{y}_2) \ .$$

*Similarly, for any subsample* $\mathbf{Z}$ *containing the parts* $X_1$ *and* $X_2$*, dominance of Aichison distance in* $\mathcal{P}$ *is*

$$\mathrm{d}_p(X_1, X_2) \geq \mathrm{d}_p(Z_1, Z_2) \ .$$

The total variance of $\mathbf{X}$ and $\mathbf{X}^\top$ are related as follows.

**Proposition B.3.** *The total variance of* $\mathbf{X}$ *by observations and parts satisfy*

$$N \ \mathrm{totVar}_o(\mathbf{X}) = D \ \mathrm{totVar}_p(\mathbf{X}) \ ,$$

*provided that variances are sums of squares divided by the number of terms, N or D. In cases where variances are estimated by dividing by* $N-1$ *or* $D-1$*, these numbers appear in the equation substituting N and D.*

*Proof.* Consider the clr of the observations

$$\mathrm{clr}_o(\mathbf{X}) = (\mathrm{clr}(\mathbf{x}_1)^\top, \mathrm{clr}(\mathbf{x}_2)^\top, \ldots, \mathrm{clr}(\mathbf{x}_D)^\top)^\top .$$

This matrix can be centred by subtracting the mean by columns. This corresponds to perturbation-subtraction of the sample centre of observations, that is

$$\mathbf{Z}_o = \mathrm{clr}_o(\mathbf{X}) - 1_N[\mathrm{clr}_o(\mathrm{Cen}(\mathbf{X}))]^\top , \tag{B.4}$$

where $1_N$ is an $(N \times 1)$-matrix of ones. The singular value decomposition of $\mathbf{Z}_o$ is

$$\mathbf{Z}_o = U_o \Lambda_o V_o^\top , \quad \Lambda_o = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{D-1}, 0) , \tag{B.5}$$

where $\lambda_i \geq 0$ are the singular values, and $U_o$ and $V_o$ are such that $U_o U_o^\top = \mathrm{I}_N$ and $V_o^\top V_o = \mathrm{I}_D$. The zero entry of $\Lambda_o$ is due to the zero-sum constraint of clr-vectors. This null singular value and the corresponding vectors (last column in $U_o$ and in $V_o$) can be suppressed since they do not influence $\mathbf{Z}_o$. Maintaining the same notation for the reduced versions of $U_o$, $V_o$ and $\Lambda_o$, the decomposition of $\mathbf{Z}_o$ is written in the same way as in Eq. (B.5). It characterizes $V_o$ as a $(D \times (D-1))$ contrast matrix and $U_o \Lambda_o$ a matrix whose $i$-th row contains the $\mathrm{ilr}_o(\mathbf{x}_i)$ with respect to $V_o$. Also, the fact that the squares of the columns of $U_o$ sum to 1, indicates that the square singular values divided by $N$, $\lambda_i^2/N$, are the variances of the ilr components in the columns of $U_o \Lambda_o$. Since the centring in Eq. (B.4) does not affect the computation of variances, the total variance of observations is

$$\mathrm{totVar}_o(\mathbf{X}) = \frac{1}{N} \sum_{k=1}^{D-1} \lambda_k^2 .$$

The same procedure (clr and centring) can be applied to $\mathbf{X}^\top$. After removing the last null singular value, the decomposition is now

$$\mathbf{Z}_p(\mathbf{X}) = U_p \Theta_p V_p^\top , \quad \Theta_p = \mathrm{diag}(\theta_1, \theta_2, \ldots, \theta_{N-1}, 0) .$$

Assuming $N \geq D$, it holds that $\theta_k = \lambda_k$ for $k = 1, 2, \ldots, D-1$ and that $\theta_k = 0$ for $k = D, D+1, \ldots, N-1$. Hence,

$$\mathrm{totVar}_p(\mathbf{X}) = \frac{1}{D} \sum_{k=1}^{D-1} \lambda_k^2 ,$$

and then

$$N \, \mathrm{totVar}_o(\mathbf{X}) = D \, \mathrm{totVar}_p(\mathbf{X}) .$$

∎

In Egozcue et al. (2018) (Appendix) and Martín-Fernández et al. (2018), it was proven that the variation matrix of observations is directly related to the square inter-distances between parts, as stated below.

**Proposition B.4.** *Let $T^o$ and $T^p$ be the variation matrices associated with the compositional sample* $\mathbf{X}$*. Consider the matrices of square interdistances $M^o$ and $M^p$ whose entries are respectively $[M^o]_{ij} = \mathrm{d}_a^2(\mathbf{x}_i, \mathbf{x}_j)$, $i, j = 1, 2, \ldots, N$ and $[M^p]_{ij} = \mathrm{d}_a^2(X_i, X_j)$, $i, j = 1, 2, \ldots, D$. They satisfy*

$$N\, T^o = M^p \ , \quad D\, T^p = M^o \ .$$

A negative property is important for discussing subcompositional coherence. In fact, the $p$-inner product is not perturbation invariant and taking into account Proposition B.1, it means that the $p$-inner product is not invariant under $o$-subcomposition.

**Proposition B.5.** *The $p$-inner product (Definition A.1) is not $p$-perturbation invariant.*

*Proof.* For two parts $X_1$, $X_2$ and $Q \in \mathcal{P}^N$, it holds

$$\langle \mathbf{p}_1 \oplus_p Q, \mathbf{p}_2 \oplus_p Q \rangle_p = \langle \mathbf{p}_1, \mathbf{p}_2 \rangle_p + \langle \mathbf{p}_1, Q \rangle_p + \langle Q, \mathbf{p}_2 \rangle_p + \langle Q, Q \rangle_p \ .$$

Consequently, in general, $\langle \mathbf{p}_1 \oplus_p Q, \mathbf{p}_2 \oplus_p Q \rangle_p \neq \langle \mathbf{p}_1, \mathbf{p}_2 \rangle_p$ . ■

The counterpart of the previous negative result is the following proposition

**Proposition B.6.** *Each component of $X_1 \ominus_p X_2$, is $p$-perturbation invariant.*

*Proof.* Let $Q \in \mathcal{O}^N$ define a perturbation for parts and consider the shifted parts $X_1 \oplus Q$ and $X_2 \oplus Q$. Then,

$$(X_1 \oplus Q) \ominus_p (X_2 \oplus Q) = X_1 \ominus_p X_2 \ ,$$

thus implying $p$-perturbation invariance, in particular each component is an invariant function (IfS). ■

All functions of $p$-differences of parts are also invariant under perturbation or, equivalently, under $o$-subcomposition. Therefore, when trying to relate two parts, say $X_1$, $X_2$, —independently of the o-subcomposition they are included in— functions of $X_1 \ominus_p X_2$ are potential candidates. The Aitchison $p$-distance $\mathrm{d}_a(X_1, X_2) = \|X_1 \ominus_p X_2\|_a$ and related functions are then serious candidates to measure co-variability between the two parts. The next proposition is a consequence of Proposition B.6.

**Proposition B.7.** *The Aitchison $p$-distance (Definition A.2) is $p$-perturbation invariant.*

## C. Are inverse or negative relations between compositions meaningful?

Many researchers, both theoretical and applied, would like to have tools to recognize inverse or negative relations between parts of a compositional sample. In a first attempt to clarify what such a negative relation is, we could loosely say that two parts are negatively related *when one part increases, while the other part decreases*. This way of thinking is

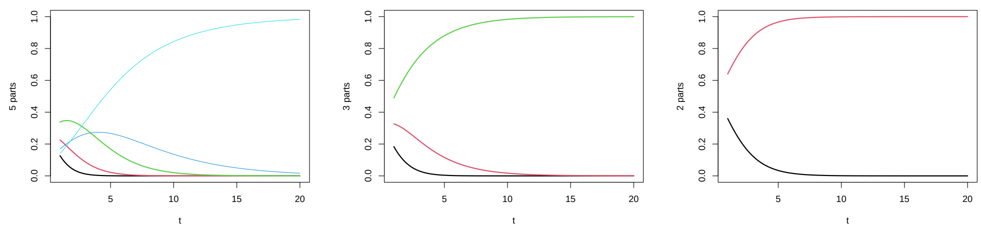


**Figure C.1.** *A five-part composition following a straight line with parameter t in the simplex is sampled in 100 data points although individual points are not shown for clarity. The left panel shows the five parts closed to 1. The middle panel represents the three parts (black, red, green), closed in the subcomposition of three parts. Closed black and red parts in a two-part composition are shown in the right panel. The monotonic relation between these three parts changes with the subcomposition.*

illusory since it strongly depends on the subcomposition in which the observations are taken. This is due to two facts. The first one is that, as mentioned in Section 4.1, taking subcomposition in the observations produces a perturbation in the compared parts which can break any monotonic behavior in the reference parts; the second one is that always one can construct an additional part that, after closure, changes the behavior of the two initial parts either to increasing-increasing or decreasing-decreasing. To illustrate this effect of closure, a 5-part compositional sample of 100 data points has been generated following a straight line in the simplex. Figure C.1, left panel, shows the five parts after closure. The parts in black, red, and green (thick lines) are taken as references. They approximately decrease jointly along the parameter $t$ of the straight line. The middle panel of Figure C.1 shows the three reference parts, now closed in a subcomposition of three parts. The parts in black and in red maintain their decreasing-decreasing relation but the black-green parts become nicely negatively or inversely related. Finally, in the 2-part subcomposition black-red (Fig. C.1, right panel) the two parts appear inversely related as mandatory in any nonconstant 2-part composition. This shows that the monotonic definition of inverse relations depends on the subcomposition in which they are observed.

A more elaborate view of the negative relation between parts $X_1, X_2$ could be to solve approximately the equation

$$X_1 = b \odot_p X_2 \oplus_p A \quad , \quad X_1, X_2, A \in \mathbb{S}^n \quad , \quad b \in \mathbb{R} \, , \tag{C.1}$$

for a minimum of $\|A\|_a$. For $\|A\|_a = 0$, there is an exact linear association (equality of compositions) between $X_1$ and $b \odot_p X_2$ and, particularly, when $b = 1$, $X_1$ and $X_2$ are proportional and compositionally equivalent (Definition 2.1). One is tempted to say that $X_1$ and $X_2$ are inversely or negatively related when, being $\|A\|_a = 0$, $b = -1$. However, the values of $A$ and $b$ depend on the subcomposition except when $b = 1$. Assuming that taking a subcomposition introduces a $p$-perturbation $P$ on the parts, the previous model is transformed into

$$X_1 \oplus_p P = b' \odot_p (X_2 \oplus_p P) \oplus_p A' = b' \odot_p X_2 \oplus_p (b' \odot_p P \oplus_p A') \quad , \quad P \in \mathbb{S}^n \ .$$

Isolating $X_1$ and substituting it by Equation (C.1)

$$b \odot_p X_2 \oplus_p A = b' \odot_p X_2 \oplus_p ((b'-1) \odot_p P \oplus_p A') \ ,$$

$$(b-b') \odot_p X_2 \oplus_p (A \ominus_p A') \oplus_p ((b'-1) \odot_p P) = \mathbf{n} \ ,$$

where $\mathbf{n}$ is the neutral element in $\mathbb{S}^n$. The values $b$, $b'$, and the compositions $A$, $A'$ will be equal whenever the term involving $P$ is neutral and this is attained for $b' = 1$ and arbitrary $P$.

As a consequence, trying to extract a negative or inverse relation from a negative value of $b$ in Equation (C.1) always depends on the subcomposition considered. Thus, this definition will never satisfy the condition of subcompositional dominance.