Revisiting the compositional data. Some fundamental questions and new prospects in Archaeometry and Archaeology

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Abstract

In this paper we examine the problem of compositional data from a different starting point. Chemical compositional data, as used in provenance studies on archaeological materials, will be approached from the measurement theory. The results will show, in a very intuitive way that chemical data can only be treated by using the approach developed for compositional data. It will be shown that compositional data analysis is a particular case in projective geometry, when the projective coordinates are in the positive orthant, and they have the properties of logarithmic interval metrics. Moreover, it will be shown that this approach can be extended to a very large number of applications, including shape analysis. This will be exemplified with a case study in architecture of Early Christian churches dated back to the 5th-7th centuries AD.

Key words: Projective geometry, homogeneous coordinates, projective points, affine points, size, composition, chemical composition, translation, shape

1 Introduction

Compositional data have generally been defined as a vector of proportions, a D-part composition **x** with strictly positive components whose sum is a constant, usually 1 (Aitchison, 1986, 2005; Barceló-Vidal and others, 2001; Pawlowsky-Glahn, 2004; Tolosana-Delagado and others, 2005; Pawlowsky-Glahn and Egozcue, 2006).

The restriction to strictly positive components is not always kept in those definitions, as it is the case, for example, in the seminal work of Aitchison (1986). In fact, strategies have been developed for zero replacement, whether they can be understood as essential or rounded zeros (see for example Aitchison and Kay, 2003 and Palarea-Albaladejo and others, 2005, and references therein).

Moreover, the above definition of compositional data has changed and nowadays expressions like ‘vector of proportions’ or the constant sum constraint are seldom employed. This shift on the emphasis given to the constraint, to the closure, is clearly related to the realization of the important role played by the scale-invariant nature of compositional data. Aitchison (1986, p. 30-33) expressed this fact relating each composition **x** to its set of basis, an equivalence class based on a multiplicative factor. Therefore, all bases in a given equivalence class, even if different in terms of size, were represented by the same composition. Possibly the most clear realization of the importance of scale-invariance can be found in the paper by Barceló-Vidal and others (2001). In that paper, the authors assert this crucial role of scale-invariance, even more important than the usual preoccupation for the unit sum constraint. Along these lines, they also define the equivalence class.

Furthermore, another basic element is the identification of the simplex as the natural sample space for closed compositional data. This space is not D-dimensional, as it could be expected for D-parts compositions, but it has one dimension less. Therefore, the simplex, but also the compositional space, is a d-dimensional one (d = D-1) (Barceló-Vidal and others, 2001). In the simplex, points are then related to its ray from the center, its compositional class.

Finally, perturbation (⊕) and powering (⊗) have become standard basic operations, that are said to correspond to translation and scalar multiplication of vectors in R^D,while Aitchison norm, Aitchison inner product and Aitchison distance have been also developed, describing the algebraic-geometric structure of the simplex (see especially Barceló-Vidal and others, 2001; Aitchison, 2005).

During this period of development, there has been an important shift of importance from the closure problem to the scale invariant property. The former was the reason for an absence of interpretable covariance structure that was at the very origin of the compositional data problem. The latter has lead to the characterization of the existing algebraic-geometric structure. All this work has achieved a strong theoretical body on compositional data, providing good results and explanations, but also good prospects for the future.

Even so, compositional data development has suffered from a large number of detractors (see Aitchison, 2005 for a summary description and references). In some cases, some aspects have been discussed on mathematical grounds, but in some other cases, the criticisms have arisen from practical aspects during the application of these analyses. In Archaeometry, Baxter can be considered as the first scholar echoing Aitchison’s work on compositional data (Baxter, 1989). However, even if accepting that compositional data analysis, as described above, cannot be criticized from a mathematical point of view, he find several practical problems and he advocates for a use of ‘standard’ techniques on the determined components (Baxter and Freestone, 2006).

The aim of this paper is to highlight several fundamental aspects of compositional data analysis in relation to projective geometries. Moreover, it is also devoted to highlight what chemical data really are. Finally, it is also devoted to develop the so called scale invariant property of compositional data. All these three aspects will contribute to strength the above proposed compositional data analysis, providing even more evidence on the impossible application of the so called ‘standard’ techniques. Along these lines, it is also the scope of this paper to extent this approach to other ‘compositional’ data sets, highlighting the existing relation with, at least, part of shape analysis. Thus, a large number of new subjects in Archaeometry and Archaeology could be addressed. Shape analysis of Early Christian churches will be used as an example.

2 Measurement and projective geometry

The problems arisen by compositional data can also be approached from the field of measurement theory, even if no measurement is really involved. In fact, the discussion of compositional data is a discussion on a multivariate representation. Thus, it is about the numerical geometrical structures encountered in analytical geometry, structures that are axiomatized by synthetic geometry. However, the geometric concept of distance is, somehow, related with measurement theory. In a qualitative way, distance is length. In a quantitative way, the interval metrics have the analytical properties of a distance (Díez, 1993).

In the following discussion we will make a quite extensive use of Suppes and others (1989) work (but also Faugeras, 1995 and Bloomental and Rokne, 1994). Let **x** be a D-dimensional vector expressing, for example, parts of a whole. Let be all components absolute values of the appropriate type. And let be these absolute values relevant. Let, finally, **x** be a point, with components as coordinates, in a vector space over R^D defined by $\langle V, +, \cdot \rangle$, where + is a binary operation with the properties of coordinate-wise addition, and $\cdot$ a function from R x V to V, with the abstract properties of scalar multiplication. Under such circumstances two vectors **x** = (3, 4, 5) and **y** = (6, 8, 10) (**x**, **y** $\in R^3$) correspond to two different points in the space.

Let now be irrelevant the absolute values of the coordinates of the former vectors, since we are just interested in the relative ones. Under such circumstances vectors **x** and **y** are equivalent, since **y** = 2 · **x**, i.e. (6, 8, 10) = (2 · 3, 2 · 4, 2 · 5), being 2 a scalar. Thus, both vectors have coordinates proportional.

As it has been shown before, when we are just interested in the relative values of the coordinates, the components, of a vector **x** we are moving away from a vector space over R^D defined by $\langle V, +, \cdot \rangle$, since the operation · does not exist anymore. Two nonzero elements of R^D are then related by scalar multiplication.

The previous fact has already been identified in compositional data analysis as the scale invariance property. However, several aspects may need further development. One of these is the concept of equivalence class of compositions or bases. If we consider that in a vector space a line having origin in **x** and direction **y** can be defined by all the elements of form **x** + t**y**, for t in R^D, it is clear that the equivalence class [**x**] = $\{t\mathbf{x} \mid t \in R^D, t \neq 0\}$ cannot be considered as a line, or ray. This is so because the scalar multiplication function does not apply in the present vector space, and then the expression **x** + t**y** is, in this geometry, meaningless. The concepts of point and direction are not independent and such equivalence class is, in fact, a point.

The geometry defined above, with no scalar multiplication, is the projective geometry. In such geometry, the equality of proportional elements of V implies a loss of one degree of freedom and, therefore, the projective geometry is one dimension less. Thus, a d-dimensional projective space arises from a d+1-dimensional vector space. In that sense, we must highlight that the usual notation in compositional data analysis of D-parts that is substantially a d-dimensional vector (d = D – 1) is, in the usual projective geometry, seen in the other way around, just to emphasize the loss of one dimension, because of the loss of one degree of freedom.

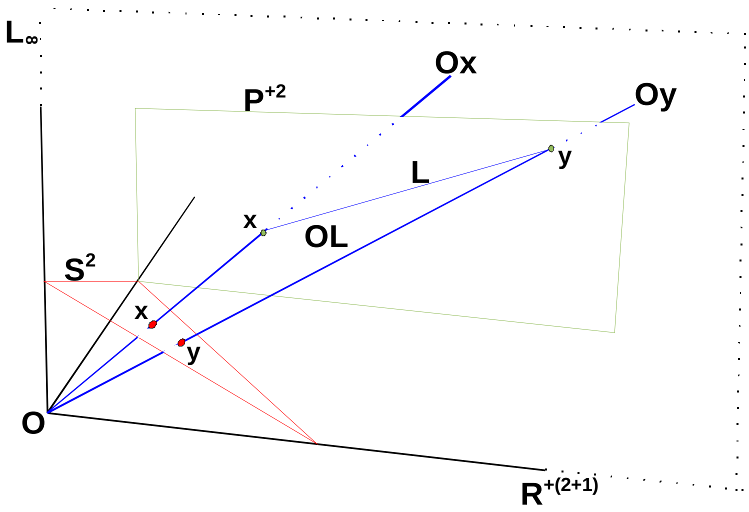
Therefore, we can say that a d+1-dimensional vector space gives a d-dimensional projective geometry, in which a projective point x in P^d is a single equivalence class [**x**] = $\{t\mathbf{x} \mid t \in R^D, t \neq 0\}$. A projective point x is represented by a d+1-dimensional vector of coordinates, or coordinate vector, **x** = $[x_1, \ldots, x_{d+1}]$ (enclosed within brackets), where at least one of the x_i is nonzero; x_i are called homogeneous, or projective, coordinates. These homogeneous coordinates are, then, the components of a d+1-part composition. Compositional data, within the frame of projective geometry, is a subset in the positive orthant R_+^{d+1}.

The following geometric representation for R_+^{2+1} (Fig. 1) is adapted after the representation from Aitchison, 1986 (among others) and that one from Suppes and others (1989). In such representation, the d-dimensional simplex is shown together with the usual projective representation. O is the origin, and Ox and Oy are two projective points. S^2 is the unit sum 2-dimensional simplex, while P^2 is the usual 2-dimensional affine plane with $x_3 = 1$. Simplex and affine points x, y in the simplex S^2 and in the plane P^2 correspond to the projective points Ox and Oy. The affine line L determined by the projective points Ox and Oy, correspond to the projective line OL. Finally, the plane L_∞, parallel to P^2 is the projective line at infinity. Figure 1 shows the relation between projective points and two especial projections. On the one hand, the S^d simplex. In that case, projective points are represented by homogeneous coordinates that have a constant sum k ($k \in R_+$):

$$S^d = \{[x_1, \ldots, x_{d+1}] : x_i \geq 0 \ (i = 1, \ldots, d+1), x_1 + \ldots + x_{d+1} = k\}.$$

The most common values for k are 1 and 100. On the other hand, the P^2 affine plane. The usual case is the one shown in Figure 1. Projective points are represented by the homogeneous coordinates $[x_1/x_3, x_2/x_3, 1]$ ($x_3 \neq 0$). Therefore, affine points are represented by the affine coordinates (x'_1, x'_2) (enclosed within parenthesis), where $x'_1 = x_1/x_3$, and $x'_2 = x_2/x_3$. The plane L_∞ is the line at infinity, and lines through 0 lying on L_∞ are points at infinity.

Figure 1: Relation between projective points, the simplex and the affine plane (for abbreviations see the text).



It is clear that the simplex is not an affine plane, but also that the one dimension less is the general loss of on degree of freedom in projective geometry. Nonetheless, the simplex is just that projective sample space in which the actual homogeneous coordinates have a constant sum, but they still are homogeneous coordinates. On the contrary, the projection in the affine plane enables to change homogeneous coordinates into affine coordinates in a d-dimensional affine space. At this point, it seems important to highlight the similarity between projection in the $x_{d+1} = 1$ affine plane and the so called additive logratio transformation *alr*.

3 Chemical analysis and logarithmic interval scales

In §2 we have seen that multivariate representations are not really involved with measurement. Even so, it is clear that every coordinate in a chemical compositional vector **x** comes from the determination of one particular elemental concentration in the sample. In that sense, it would be worth asking which kind of measurement do we face when determining these concentrations.

To answer the above question first we should focus in one important point, i.e. matter is a classificatory concept. In fact, all matter is classified into different atoms in an exhaustive classification, with mutually excluding classes, which are systematically based on the number of protons (see for example, Díez and Moulines, 1999, p. 102-103). This classificatory base of matter is one of the characteristics of chemistry itself, a discipline that has been described as a '…classificatory science of materials which works with experimental methods…' (Schummer, 1997, p. 308). Besides, it must be acknowledge that another important peculiarity of chemistry is its abstraction from form, size and mass. This is achieved by three main procedures: standardization, forming intensive quantities, and relative quantities (Schummer, 1997, p. 311-312).

Once we are aware of the previous stated facts, it is easy to see that chemical analysis is not really involved in measuring, but in enumerating, or counting, the number of each type of atoms in a sample. This counting is not expressed in absolute numbers, i.e. in the total number of atoms existing in the whole sample or in the whole individual under study. On the contrary, the result, by any of the three main procedures pointed above, will be given in relative numbers (usually in % or ppm). Thus, several remarks should be now considered: 1- elemental concentrations are frequencies of nominal or categorical classes (atoms) of a classificatory concept (matter), 2- chemistry is usually interested not in frequencies, but in relative frequencies. Therefore, three conclusions must be retained by now: 1- it is misleading to talk about absolute values or concentrations when we are considering the components of a chemical compositional vector, since they express relative, not absolute, concentrations, 2- along these lines, *alr* or *clr* transformed values in compositional data analysis should not be called relative values, because non transformed components do are these relative values, 3- and more important, chemical data are relative frequencies of atoms and therefore their natural expression is in elemental atomic percentages.

Determination of elemental concentrations is the process of identification of different types of atoms, and the enumeration of the identified atoms per type. The result is the relative frequencies for the identified atoms, i.e. elemental atomic percentages. Even so, atoms are not really counted. Analytical chemistry is the branch of chemistry that deals with this quantitative determinations (for our interests, we can now ignore the qualitative determinations, and even the semiquantitative ones). Without entering into further considerations, we can say that nowadays the determinations are, usually, based on instrumentation of some sort that uses physical principles to identify atoms in the sample. Besides, concentrations are derived from the recorded signal, usually the absorption or emission lines in a spectrum (see, for example, Pollard and others, 2007). These procedures in analytical chemistry do are measurements. However, the conversion of such measured values into estimates of relative frequencies of atoms is achieved thanks to the constant (or constant under several considerations) properties of atoms. Therefore, estimation of relative frequencies can be regarded, finally, as an indirect process of counting.

A further crucial realization about chemical concentrations is that they are not always given in atomic percentages. On the contrary, in most fields of application it is a common practice to express the results in weight percentages, by using the relative atomic mass or atomic weight, i.e. the average of the atomic masses of all the chemical element's isotopes weighted by isotopic abundance. Moreover, atomic percentages and weight percentages are also expressed in oxides, usually by stoichiometric combinations with oxygen. It is then clear that the components attached to a composition are the result of a subjective choice, based on tradition or other factors, but they are not the only possible expression for the same chemical concentrations in a given sample.

We can see this point in a short example. Let $\mathbf{x} = [20, 30, 40]$ be a compositional vector of three parts Fe, Ca and Si, with elemental atomic percentage components of a given sample A. The results can be reported as in Table 1.

Table 1. Elemental atomic percentage concentrations for sample A.

Element	*Atomic %*
Fe	20
Ca	30
Si	40
Total	100

If a researcher would prefer to express the same determined elemental concentrations on atomic percentages in oxides, therefore the researcher would be obliged to multiply every component by a fixed factor, the proportion of the atoms in the chosen oxide, and reporting the results back to percentages, i.e. using the closure operation. This change is shown in Table 2.

Table 2. Oxide atomic percentage concentrations for sample A.

Element	*Atomic %*	*Factor*	*Closure*	*At. % oxide*	*Oxide*
Fe	20	$(2/5)^{-1}$	50	21.74	Fe_2O_3
Ca	30	$(1/2)^{-1}$	60	26.09	CaO
Si	40	$(1/3)^{-1}$	120	52.17	SiO_2
Total	100		230	100	

Another usual option is to express the results in Table 1 as elemental concentrations in weight percentages. In that case, the researcher would multiply the elemental atomic percentages by a different set of factors, the atomic weight of the elements, and then closing back the components. This is shown in Table 3.

Table 3. Elemental weight percentage concentrations for sample A.

Element	*Atomic %*	*Factor*	*Closure*	*Weight %*
Fe	20	55.847	1116.94	32.44
Ca	30	40.08	1202.4	34.93
Si	40	28.086	1123.44	32.63
Total	100		3442.78	100

In our final case, the researcher could be interested in reporting the elemental atomic percentages as weight percentages, but for oxides. In such case, the fixed factors would be a combination of the proportion of the atoms in the chosen oxide and their atomic weights. As in previous cases, the data would be finally closed. Table 4 shows this case.

Table 4. Oxide weight percentage concentrations for sample A.

Element	*Atomic %*	*Factor*	*Closure*	*Wt. % oxide*	*Oxide*
Fe	20	0.695504^{-1}	28.76	18.40	Fe_2O_3
Ca	30	0.7147698^{-1}	41.97	26.85	CaO
Si	40	0.4675234^{-1}	85.56	54.75	SiO_2
Total	100		156.29	100	

The final purpose of this example is to highlight that the same elemental chemical concentrations can be expressed in, at least, four different common ways. Thus vectors $\mathbf{x}$ = [20, 30, 40], $\mathbf{x}'$ = [21.74, 26.09, 52.17], $\mathbf{x}''$ = [32.44, 34.93, 32.63], and $\mathbf{x}'''$ = [18.40, 26.85, 54.75] should be considered as equivalent, even if expressed in what could be assumed as coordinates determined in different scales. It is also obvious that the vectors $\mathbf{u}^{(1)} = [(2/5)^{-1}, (1/2)^{-1}, (1/3)^{-1}]$, $\mathbf{u}^{(2)}$ = [55.847, 40.08, 28.086], and $\mathbf{u}^{(3)} = [0.695504^{-1}, 0.7147698^{-1}, 0.4675234^{-1}]$ of transformation factors can be identified with the perturbing vectors in the operation of perturbation.

The previous example makes clear that if the differences of intervals for two samples A and B expressed in different kinds of scale (for example, elemental atomic percentage and oxide weight percentage) must be constant, it is necessary for the operation of perturbation to be invariant under such kind of change of scale. This is the same as saying that perturbation should be the translation within the group of transformations. However, translation is an additive operation, while perturbation is a multiplicative one. This result leads to two different conclusions:

1- In compositional data analysis we are not dealing with interval metrics having the analytical properties of a distance, but with logarithmic interval metrics. Therefore, different kinds of coordinates can be seen as belonging to exponential transformations of the type $f(x) = ax^n$ ($a, n \in R^+$), with the special case of n = 1, being a the multiplicative factor. These transformations take the form of $\ln(f(x)) = \ln(x) + \ln(a)$, and they keep invariant the values $\ln(f(x)) - \ln(f(y)) / \ln(f(z)) - \ln(f(w))$. By extension, this is also true of any fixed perturbation.

2- The fixed exponential n in the previous exponential transformation of the type $f(x) = ax^n$ ($a, n \in R^+$), with the special case of a = 1, is the powering operation.

At this point, it is important to recall the projection of the projective points onto the $x_3 = 1$ P^2 affine plane shown in Figure 1. We have already pointed out the similarities between this projection and the *alr* transformation. The main difference between them is that the *alr* transformation takes the logarithms of $x_3 = 1$ P^2 affine coordinates. The original reason for that was the need for symmetry in the rations. Even so, as it has been shown, since compositional data correspond to a multiplicative model, the appropriate metric is that of logarithmic interval one. Therefore, taking logarithms is necessary from measurement theory in order to have an appropriate projection.

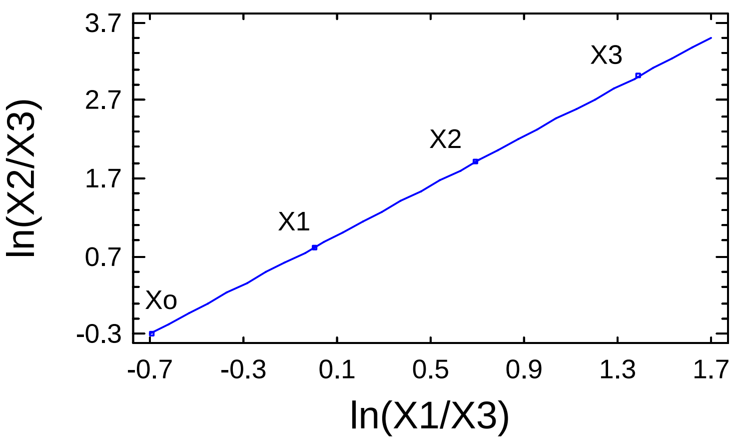
So, if a fixed perturbation operation arises naturally as a translation in exponential transformations, in a change of measurement scale for the coordinates, this operation can also model changes, not necessarily fixed, related with, for example, weathering processes (see for example, Aitchison and Thomas, 1998; Buxeda, 1999).

Considering the projective geometry and the multiplicative model, we can model these changes, these perturbations, in the affine space. If we take the three parts compositional vector $\mathbf{x}_0 = [20, 30, 40]$ and we induce three perturbation cycles, with the perturbing vector $\mathbf{u} = [4, 6, 2]$, then we have $\mathbf{x}_3 = \mathbf{x}_0 \oplus (3 \otimes \mathbf{u})$. First, let's take the $x_3 = 1$ affine coordinates from the $\mathbf{x}_0$ homogeneous coordinates, i.e. $x_0 = (0.5, 0.75)$. Since for a given projective point we can use any vector as homogeneous coordinates, let's take the affine coordinates, with $x_3 = 1$, as the new homogeneous coordinates $x_0 = [0.5, 0.75, 1]$. Then, because we are dealing with logarithmic interval metrics, let's take the logarithms of the previous homogeneous coordinates $alr(\mathbf{x}_0) = [-0.693147, -0.287682, 0]$. Now, let's do the same procedure for the perturbing vector. This gives an affine perturbing vector $\mathbf{u} = (2, 3)$, which can be used for a new set of homogenous coordinates for the perturbing vector $\mathbf{u} = [2, 3, 1]$. Now, we can use a matrix operation for translation in the affine space with $\mathbf{x}' = \mathbf{x} + \mathbf{u} = \mathbf{xI} + \mathbf{u}$, where $\mathbf{I}$ is the identity matrix. In the homogeneous coordinate system this can be done in three successive steps, adjusting the values of $\mathbf{x}$ at every step, but it could be done in one single operation as follow,

$$\left[x_1', \ x_2', \ 0\right]^T = \left[-0.693147, \ -0.287682, \ 0\right]^T \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 \cdot 0.693147, & 3 \cdot 1.09861 & 0 \end{pmatrix}.$$

The result of these successive perturbations can be seen in the affine plane in Figure 2.

Figure 2: Initial composition and three successive perturbations as projected in the affine plane.



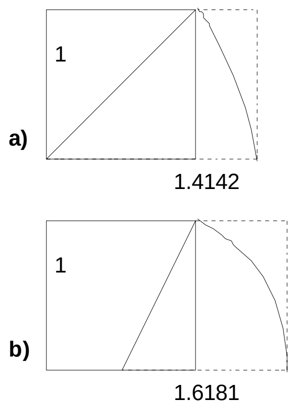
Thus, before finishing this section, it is important to highlight that compositional data are an especial case in projective geometry, whose vector space is the positive orthant, following a multiplicative model with a logarithmic interval metrics.

3 Shape analysis, and projective geometry

In the previous section we have seen how compositional data are a particular case in projective geometry. The case of compositional data is a clear case in which components are parts of a whole. However, considering as a starting point that we are dealing with parts of a whole is misleading. In fact, projective geometry is not really on parts of a whole, but on projective points, i.e. on proportional equivalence classes in a vector space without · as a function from R x V to V, with the abstract properties of scalar multiplication. Therefore, any case of proportional equivalence classes, limited to the positive orthant, and following a multiplicative model can, and should, be dealt with the theoretical and methodological framework that is being developed for compositional data.

A typical case is that of shape analysis. Let's consider, for example, that we are studying rectangles. And let's consider that we have two different models. On the one hand (Fig. 3, a), rectangles in a proportion based on the irrational number of $\sqrt{2}$ (i.e. $2^{0.5} \approx 1.4142$). Such rectangles are based in a square with side 1, whose diagonal has been projected to one side in order to get the rectangle. Therefore, if one side is 1, the other one is $2^{0.5}$. Furthermore, all rectangles in such projective point have a proportion of $2^{0.5}$ when the longest side is divided by the shortest one. On the other hand (Fig. 3, b), rectangles in a proportion based on the irrational number Φ (i.e. the Golden Section; $\Phi \approx 1.618$) (see for example, Ghyka, 1978). In that case, starting with the square of side 1, the line that goes from the centre of the side to the corner is projected. Thus, if the short side of the rectangle is 1, the longest one is 1.618. And all rectangles belonging to this equivalence class have the short side in a proportion of Φ with the long one. It is then clear that this kind of rectangles have no free lengths for their sides, having one dimension less and being a typical case of projective geometry.

Figure 3. a) rectangles whose sides are in proportion of √2. b) rectangles whose sides are in proportion of Φ.



In this case, it is clear that changing a rectangle from the √2 type to the Φ type would require, for example, multiply the short side by 1 and the long one by (1.6181/1.4142). Thus, **u** = [1, 1.6181/1.4142] would be such a perturbation vector. Then, we are clearly dealing with proportional equivalence classes in the positive orthant, following a multiplicative model.

To provide an example of application to a real archaeological case study, let's consider the Early Christian Churches, dating back to the 5th-7th century AD. The present case study is an update of a previous study, and some references will not be given now (for details, see Gurt and Buxeda, 1996). The objective of the study is to compare the Early Christian Churches in the eastern part of the Iberian Peninsula and the Balearic Islands with those existing in northern Africa and the Levant, in order to identify different types of designs. The main objective, however, is not the existing build spaces, but the proportional systems underlying the measures of different parts. Thus, it is out of interest whether the apse has two chambers, one to each side, or it is just extant. In the former case, the head of the Church would look like the one reproduced in Figure 4, i.e. as a rectangle. On the contrary, an extant apse would look like the usual churches of nowadays, breaking the rectangular shape.

The fact that ancient buildings, and for sure those of the Greek and Roman traditions, are based on proportional systems is well known. This is even more the case for the *aedes sacrae*, i.e. the religious buildings. One of the best sources is found in Vitruvius' ten books on architecture. This Roman architect, who lived in the 1st century BC, wrote those books not for other architects, but just as general book for the emperor Augustus. Even so, he clearly states the need for such a system of proportions:

"*Aedium compositio constat ex symmetria, cuius rationem diligentissime architecti tenere debent. Ea autem paritur a proportione, quae graece analogía dicitur. Proportio est ratae partis membrorum in omni opere totoque commodulatio, ex qua ratio efficitur symmetriarum. Namque non potest aedis ulla sine symmetria atque proportione rationem habere compositionis, nisi uti [ad] hominis bene figurati membrorum habuerit exactam rationem*" (Vitruvius, III, 1, 1) (Gros, 1990, pp. 5-6).

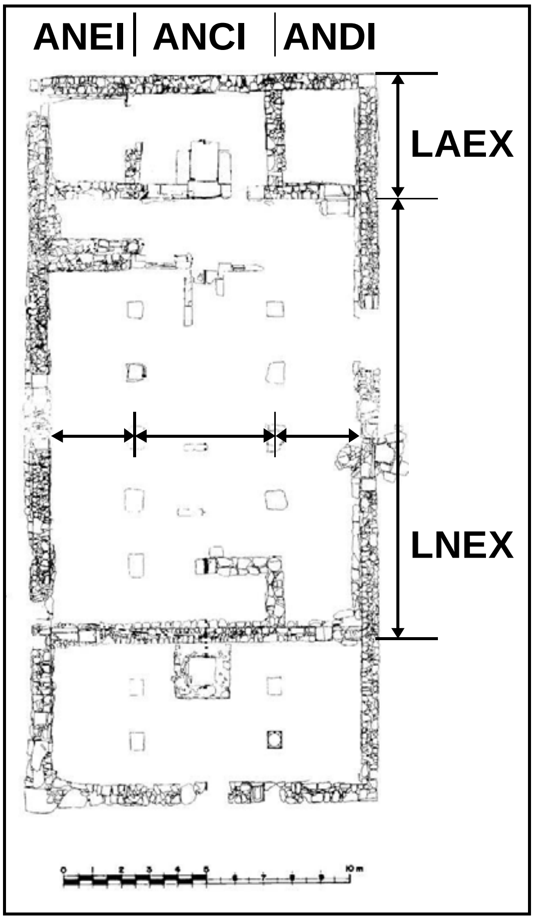
These principles seem to have been adopted in the Early Christian churches. Here, the information is less evident, but can also be identified for example in the letters written by the 4th century AD bishop Gregory of Nyssa:

"*Fiat autem ex computatione perfectioni tuae notum, quantam dimensionem universum opus computabitur. (...) Altitudinem autem in his etiam proportio latitudinis efficiet.*" (Gregory of Nyssa, *Letter XXV*) (Migne (Ed.), 1863, cols. 1093-1100).

Unfortunately, the information is very scarce and the proportional systems in use, its design and application, as well as their philosophical and liturgical implications, are still not well understood, and the research need to be pushed forward.

In the present case, the study has been based on five different measures (Figure 4). Three of them (ANEI, ANCI, and ANDI) account for the width of the building, and the separations are established in the two column lines that divide the space in three naves, the central one and the two aisles. The other two (LAEX and LNEX) account for its length. The division is established in the separation of the apse and the nave, the space for the public. In some churches, like in El Bovalar (Seròs, Lleida) (Figure 4), the building is extended with other spaces for different purposes. In that case, the space corresponds to the baptistery, placed in a separate space because the non-baptized were not allowed to go into the church. Even if these spaces have not been considered, it must be noticed that the identification of such spaces as something different is not always clear. This is especially the case for the so called churches with opposite apses, one at every end of the building. Finally, it must be taken in consideration that most of these buildings have not been well preserved. Therefore, it is not always apparent that measurements are taken as appropriate. This is especially the case for those churches that have been transformed during their ancient period of use. For example, the church of Es Cap des Port (Fornells, Menorca) was left with only the central nave (ANCI), while the aisles were transformed in several rooms used as burial environments.

Figure 4: El Bovalar, with indication of the considered measures (in cm).



Thus, 7 churches from the Iberian Peninsula and the Balearic islands have been studied (Table 5, from Casa Herrera to El Germo). Casa Herrera and El Germo have been duplicated because of the difficulties in the identification of the spaces under study. As already stated above, both churches exhibit opposite apses. Moreover, 28 churches from the Levant have also been considered (Table 5, labelled with SI and P). Finally, 6 churches from northern Africa have also been included (Table 5, labelled with AF). The values contained in this Table 5 describe, up to a certain degree, these churches in terms of size and composition, i.e. system of proportions or shape. Since we are just interested in composition, these data can be regarded just as homogeneous coordinates.

Table 5. Studied churches and measures.

Church	Label	LNEX	LAEX	ANEI	ANCI	ANDI
Casa Herrera 1 A	CH1A	2145	630	385	590	395
Casa Herrera 2 A	CH2A	1640	630	385	590	395
El Bovalar	BOVA	1601	421	310	490	296
Son Peretó	SONP	1898	488	336	534	370
Vil.la Fortunatus	VF02	1616	502	318	634	336
Son Bou	SONB	1606	640	310	456	310
Es Cap des Port	FOR1	1775	523	253	683	295
El Germo 2 A	GO2A	1700	395	210	360	200
El Germo 2 B	GO2B	1475	395	210	360	200
Sei Slelman	SI01	2675	515	395	880	395
Narab Sams	SI02	2105	425	300	625	320
Kafr Nabo	SI03	2497	483	390	811	390
Kfellusin	SI04	1588	420	315	604	291
Gerade	SI05	1615	345	285	612	273
Batuta	SI06	1616	360	267	653	268
Sergible	SI07	1919	472	330	705	340
Darqita	SI08	2185	552	333	795	345
Kfeir DarCazze	SI09	2030	435	291	648	286
Baqilha	SI10	1580	430	295	615	280
Faferlin	SI11	2420	410	360	720	368
Qa1'at Kalota	SI12	2179	490	337	820	353
Ruweiha	SI13	3135	885	415	985	415
Dehes	SI14	1943	444	406	685	381
Berris North	SI15	1334	413	240	655	240
Behyo	SI16	1918	455	310	680	310
Ba'uda	SI17	1514	440	280	635	280
Gubelle	SI18	1555	365	317	680	324
Kimar	SI19	2515	440	371	756	406
Sugane	SI20	1732	372	317	626	352
Sinhar	SI21	2171	325	225	517	313
Burg Heidar	SI22	2006	410	380	725	360
Bettir	SI23	1367	335	240	440	240
Bafetin	SI24	1520	385	360	590	330
Brad	SI25	3772	552	590	1054	592
Kalota	SI26	1819	417	297	691	342
El Ksefe North	P275	1955	400	320	600	320
Ein Hanniya	P270	1360	400	265	670	265
Sbetila I	AF01	2520	560	445	700	420
Sbetila IV	AF02	2820	650	360	635	330
Tebessa	AF03	3670	960	520	940	505
Naidra II	AF05	1730	650	310	700	310
Henchir Goraat ez Zid	AF06	1570	475	280	400	290
El Asabaa	AF07	2340	585	530	680	550

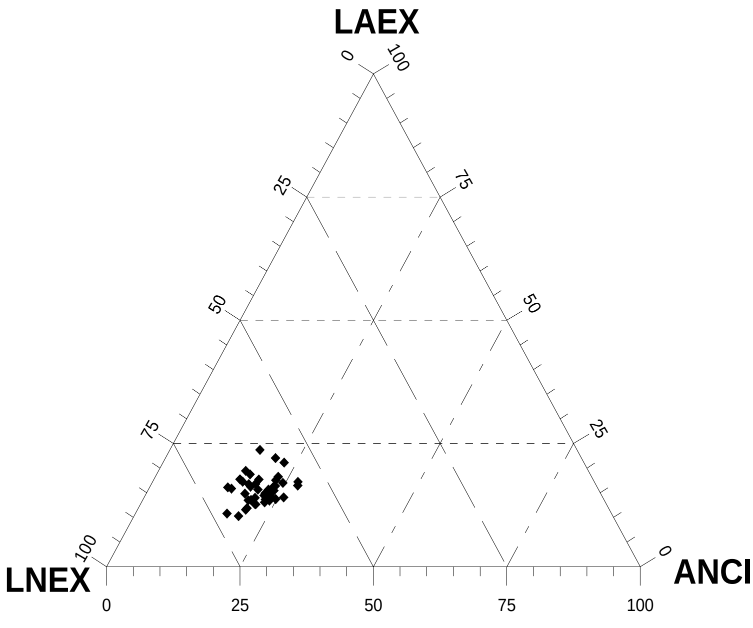
As a first exploratory tool, the variation matrix is calculated (Table 6). This variation matrix is the standard one introduced by Aitchison (1986). It shows all logratio variances and the total variation (vt). The value $\tau_{.i}$ corresponds to the value tr($\mathbf{\Sigma_i}$), i.e. the trace of the variance-covariance matrix of the *alr* transformed data by using the i^{th} component as divisor. Moreover two other values enable to measure two problems arising from this *alr* transformation (Buxeda, 1999). On the one hand, the variation matrix will then allow us to measure the variability linked to the component used as divisor in the *alr* transformation. In that sense, vt/$\tau_{.i}$ is the percentatge of $\tau_{.i}$ explained by the vt, while the subtraction 1-(vt/$\tau_{.i}$) is the variability imposed on $\mathbf{\Sigma_i}$ by the component x_i due to its special role in this asymmetric transformation *alr*. On the other hand, it must be stressed that the *alr* transformation impose a distortion because of the relations existing between all components and the component used as divisor. This distortion can be measured with a correlation coefficient $r_{v,\tau.}$ between the τ_{ji} (j=1,...,i-1,i+1,...,d+1) values in the i^{th} column and the $\tau_{.j}$ (j=1,...,i-1,i+1,...,d+1) values of the totals of the other columns, 1 being the value for no distortion.

Table 6. Variation matrix of the data in Table 5.

	LNEX	LAEX	ANEI	ANCI	ANDI
LNEX	0	0.048495	0.030029	0.039236	0.026186
LAEX	0.048495	0	0.041613	0.062535	0.045193
ANEI	0.030029	0.041613	0	0.032683	0.005548
ANCI	0.039236	0.062535	0.032683	0	0.030451
ANDI	0.026186	0.045193	0.005548	0.030451	0
$\tau_{.i}$	0.143946	0.197836	0.109873	0.164905	0.107378
$vt/\tau_{.i}$	0.502924	0.365928	0.658886	0.439003	0.674195
$r_{v,\tau}$	0.987444	0.912614	0.953083	0.987019	0.987490
vt	0.072394				

The observation of this variation matrix enables to realize that the variable with a higher variability is the length of the apse ($\tau_{.i}$ = 0.197836). Obviously, if the studied churches do correspond to different systems of proportions, this variable will be the one with a highest degree of discrimination. At the opposite side, we have the width of the two aisles ($\tau_{.i} \approx 0.1085$, in both cases), suggesting that the width of the aisles will not have a so important discriminant power. It is also important to point that the value $\tau_{ANEI,ANDI}$ (= 0.005548) is, by far, the lowest in all the variation matrix. Obviously, this value is due to the fact that both aisles are, in principle, of the same size and, therefore, both values are almost the same in all churches. In this respect, the value $\tau_{LAEX,ANCI}$ (= 0.062535) is the highest one. Of course, this is a clear indication that the relation between the length of the apse and the width of the central nave is the architectural element that could help the most in differentiating the existing systems of proportions. Moreover, this relation also agrees with LAEX and ANCI, being the two variables with the highest $\tau_{.i}$ values. Finally, the length of the nave is the third variable in terms of variability, and its highest value is that of $\tau_{LNX,LAEX}$ (=0.048495), again a high variability related to the length of the apse.

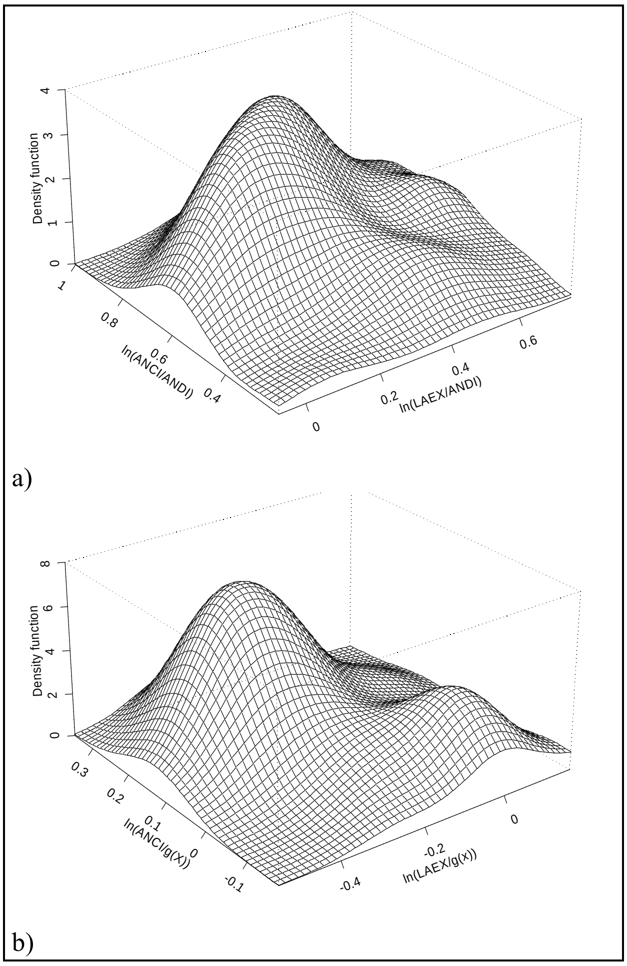
Figure 5: Ternary diagram representing all the studied churches.



As it can be seen in Figure 5, once we consider the data in Table 5 as homogeneous coordinates, we could represent them in any new set of homogeneous coordinates; since the whole set of possible homogeneous coordinates represent the same projectives points. In this sense, we can select the three variables LNEX, LAEX, and ANCI, the ones carrying the highest variability, and we can select as a new set of homogeneous coordinates the ones subject to the constant sum of 100. This representation can be, at first, senseless from an intuitive point of view, since we are not dealing with parts of a whole. But this is a misleading interpretation of what homogeneous coordinates of projective points are. Thus, it is possible to represent these churches in such a ternary diagram as Figure 5, and to use all tools developed for the study of compositional data in such ternary diagrams. For our present case study, it is now important to indicate that all churches show not really big differences, something that could be expected after the low total variability (Table 6), but still they do not seem to form a compact cloud of points.

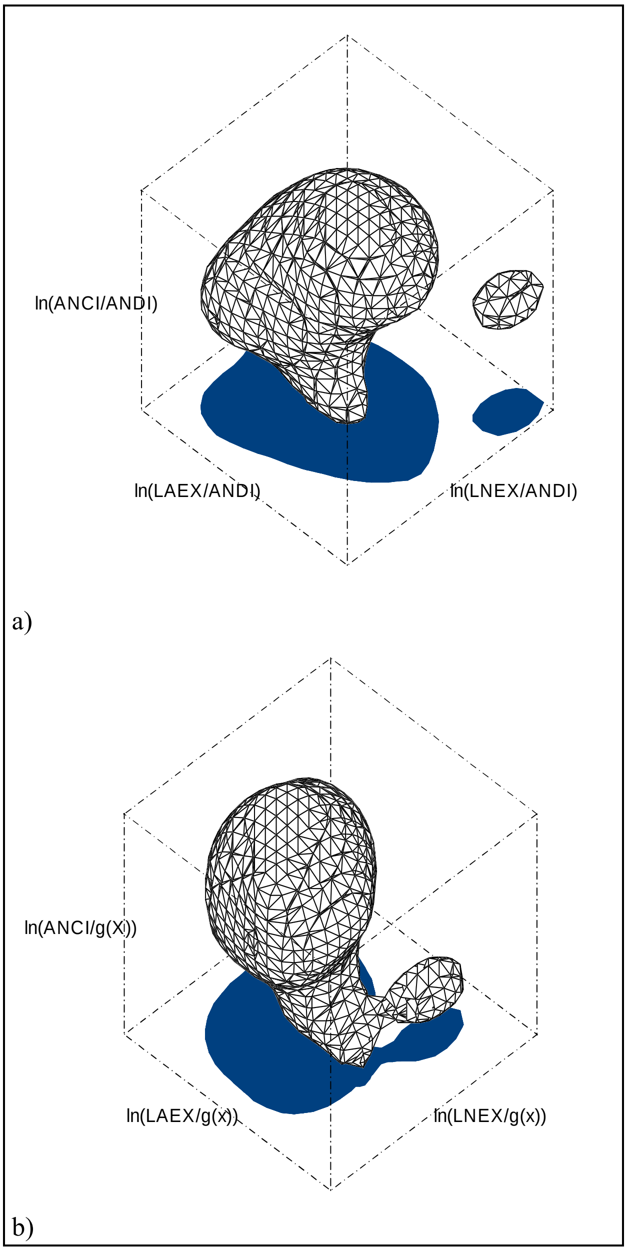
Considering that the two variables carrying the highest amount of variability are LAEX and ANCI, the length of the apse and the width of the central nave, we can further explore this variability with the use of bivariate Kernel density estimates (Bowman and Azzalini, 1997) with S-Plus (MathSoft, 1999). Here, and in what follows, we will use two different types of projection. On the one hand, the *alr* transformation, because of its similarities with the $x_{d+1} = 1$ affine space transformation. On the other hand, the centred logratio *clr* transformation (see, for example, Aitchison, 2005). In the former case (Fig. 6, a) a wide maximum can be seen that relates, somehow, medium-high *alr*-values of the width of the nave, with low-medium *alr*-values of the length of the apse. Moreover, two small maximums can be also seen relating medium-high *alr*-values of the length of the apse, with lower *alr*-values of the width of the central nave, in comparison with the wide maximum. In the *clr* transformation (Fig. 6, b), the picture is slightly different, since it exhibits two clear maxima. One of them, the larger one, relates large *clr*-values of the width of the central nave with low *clr*-values of the length of the apse. The second one, which is clearly smaller, relates low *clr*-values of the width of the central nave with large *clr*-values of the length of the apse.

Figure 6: *Bivariate Kernel density estimate plots for variables LAEX and ANCI. a) projected through alr transformation. b) projected through clr transformation*.



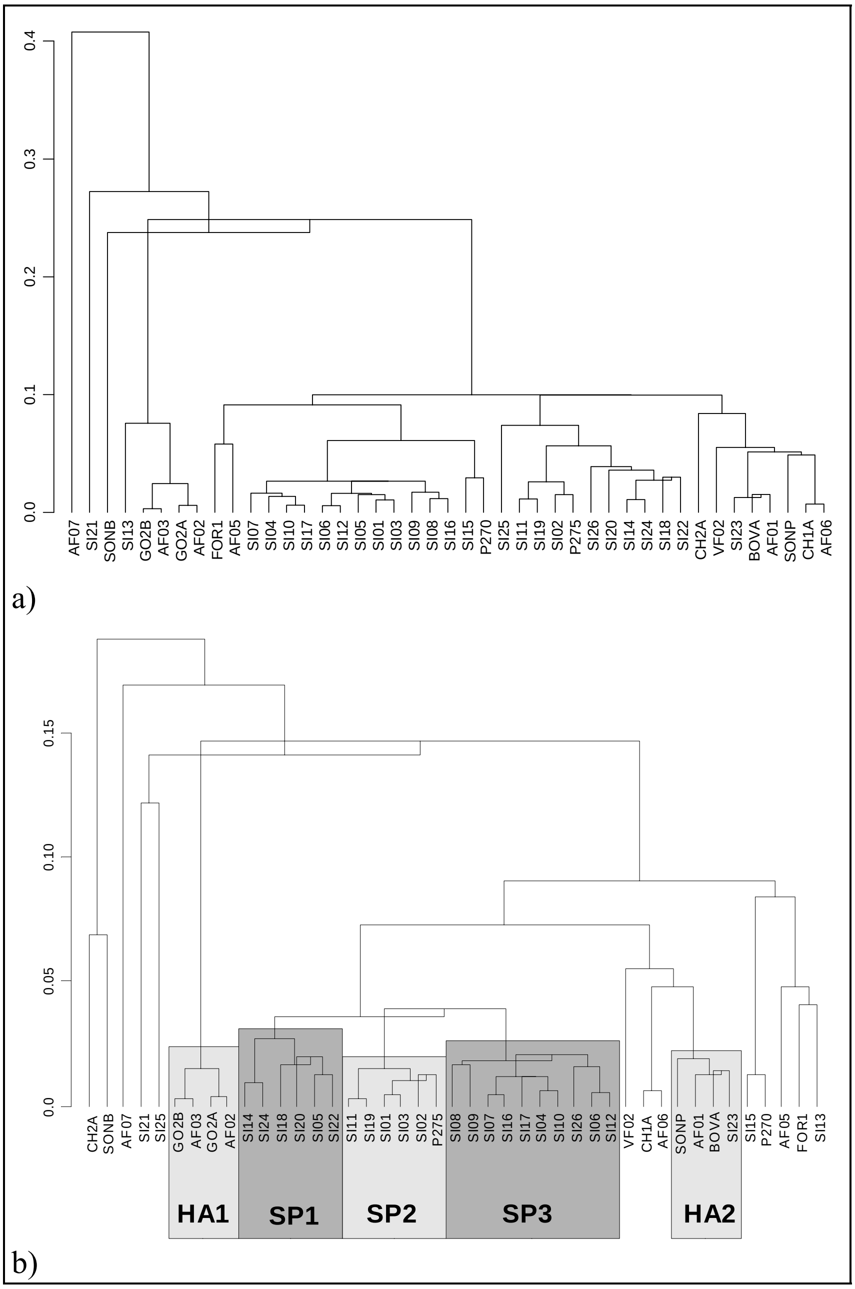
If now we decide to include the third most variability carrying variable, LNEX, the length of the nave, we will obtain somehow similar pictures when performing 3-variate Kernel density estimates. With *alr*-values (Fig. 7, a), the previous picture of a wide large maximum and two more small maxima is still recovered. However, one of these small maxima is falls now clearly apart because of the high *alr*-values of the length of the nave. Something similar happens with the *clr*-values (Fig. 7, b). Now, the large maximum can be seen as a quite consistent spherical group, but the small maximum is now divided in at least two clear distinct tendencies because of the existence of several high *clr*-values for the length of the nave.

Figure 7: *Three-variate Kernel density estimate plots for variables LAEX, ANCI, and LNEX. a) projected through alr transformation. b) projected through clr transformation.*



A final explorative tool is the use of the cluster analysis. In this application, it is clear that a metric is induced by the use of Aitchison distance on the *clr*-values. However, when calculating a distance just with the *alr*-values, using only those of the projection with variable ANDI as divisor, we are not inducing such a metric (see, for example, Pawlowsky-Glahn and Egozcue, 2006). However, it can still be used in order to measure similarities in this particular projection. Since now we are also interested in what happens in this projection on the affine space, we will also perform cluster analysis on these affine coordinates. For the *alr*-values, the dendrogram resulting by using all the variables *alr*-transformed, with ANDI as divisor, performed using S-Plus with the squared Euclidian distance formula and the centroid agglomerative algorithm can be seen in Figure 8, a. For the *clr*-values, the dendrogram resulting by using all the variables *clr*-transformed, performed using S-Plus with the squared Aitchison distance and the centroid agglomerative algorithm can be seen in Figure 8, b.

Figure 8: Dendrogram resulting from cluster analysis. a) on the *alr*-values. b) on the *clr*-values.



The results show the existence of a quite large number of different groups and non classified individuals. Moreover, both dendrograms show remarkable similarities. If we focus now our attention to the *clr*-transformed data (Fig. 8, b), it is easy to identify three groups labelled SP1, SP2, and SP3 that include most of the churches from the Levant. These groups are merged at a closed ultrametric distance and they are the main responsible for the large maximum in Figure 6, b and in Figure 7, b. On the other hand, the groups HA1 and HA2 include churches from the Iberian Peninsula and Balearic Islands, and northern Africa. These two groups were responsible for the small maximum in Figure 6, b, and for the two small groups in Figure 7, b. It is then clear, that the structure underlying the studied churches is based in a two different models, in a wide sense, that can be identified with an eastern model, and a western one. These two main models offer, however, a significant variability that needs to be further explored. Besides, some points of interest arise. First, in group HA2 is classed the eastern church of Bettir (SI23). The space of this church is organized, in terms of liturgical elements, in a similar way to those churches classed in the eastern model. Even so, from an architectural proportion system, it is clearly related to the western one. A second point of interest is the existence of several churches not well classed. Some of them merge with group HA2 and should be considered as close to the western model. For example, the church of Villa Fortunatus (VF02) was not built as a church from the very beginning. Instead, it corresponds to several chambers of a rural Roman villa that were transformed in a small church. Then, it seems clear that even if the new building was partly determined by the existing one, the adaptation was made in order to obtain what was seen as a typical western church. Another group of churches that have not been classed can be seen at the right hand side of the dendrogram. These churches have intermediate characteristics between the two models. Among them, the church of Es Cap des Port (FOR1), located in Minorca, is a clear example of western church that is based on the eastern model. The fact that this church has suffered several changes and that it is difficult to identify the original design must be the responsible for this intermediate like classification. Finally, it is important to highlight the fact that the five churches at the left hand side of the dendrogram do not correspond to any defined model. Instead, they seem to be special cases that can only be explained in a one to one basis, even as members of different models.

4 Conclusions

As it has been shown, we believe that what is called compositional data analysis is the special case in projective geometry in the positive orthant whether the coordinates have the properties of logarithmic interval metrics, since the coordinates behave as they belong to exponential transformation groups.

The cases that can be account for are numerous and of very different nature. They can include all coordinates based on frequencies, but also parts of a whole in a wide sense. The latter can include non evident parts of a whole, as it is the example shown here with different measures of the churches. This is so, because the important thing is that all parts, all coordinates, are not free, because they belong to a given projective point, or equivalence class, and therefore one of their dimensions is loss. In all these situations, the coordinates can include two types of information, size and composition. If size is relevant, then, the problem is not of a compositional nature and it is not a projective geometry case. However, if size is not important and relevant information is in composition, then we are dealing with a projective geometry case.

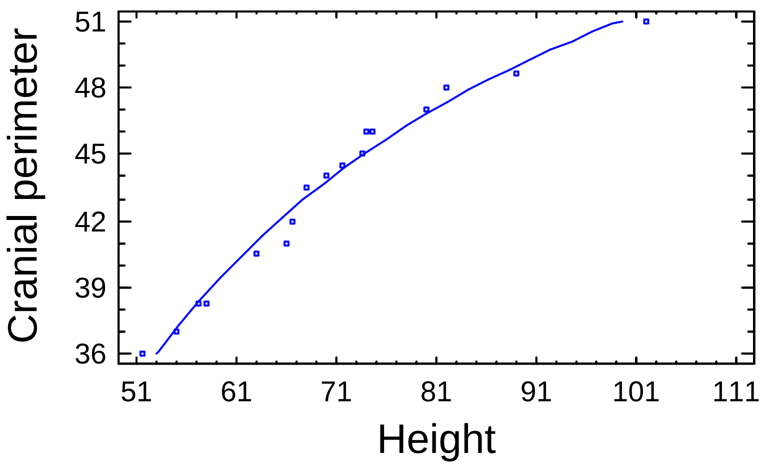
Besides, there are a large number of situations where the coordinates are relative frequencies, as it is the case for chemical data. In such cases, size is not preserved anymore and the only possible study is in terms of composition. In our opinion, the term relative value should be used to describe this coordinates, while the term absolute value should be preserved for those coordinates that include information on size.

Whether the values of the coordinates are absolute of relative, it is important to realize that all of them are homogeneous coordinates in a projective geometry. In that sense, it is important to realize that the simplex is still in the projective geometry, even if it is the particular case in which the sum of the coordinates adds up to a constant.

Those homogeneous coordinates can be, then, frequencies, relative frequencies and measures. Chemical data are a special case, since they are, finally, frequencies, or relative frequencies. However, the way those frequencies are counted is an indirect method of counting, and the discrete particles or compounds being counted are observed through their physical characteristics and properties, which can be considered fixed at the level of interest. Because of that, the results are not given necessarily as relative frequencies of counts of such particles or compounds. Usually, they are also expressed as, for example, weight. Even so, this should be understood as the use of different equivalent scales, and this should not change the results in terms of composition.

In Archaeology and Archaeometry the list of subjects that should be considered as compositional data analysis cases is a long one. It includes chemical analysis, but also the study of assemblages, like pottery. The latter case, however, is a very especial case, since the usual state of the recovered archaeological material is fragmentary and uncomplete, imposing difficulties in the identification of frequencies. Furthermore, there are also a large number of cases that could be classified as shape studies, like the proposed case of models of proportions in Early Christian churches. As it can be easily understood, however, shape analysis in terms of compositional data analysis can not readily be applied for those situations affected of allometry. This can be clearly seen with the example of our older son Jaume, a 4 years old child who is happily growing up. If we look to his evolution, we can see that his cranial perimeter and his height do not develop at the same rhythm (Figure 9). The fitted model do not correspond to a linear one, but to a reciprocal-X (Y = a + b/X). Under these circumstances different bones of several living organisms belonging to the same taxon could not be identified as the same projective point. Facing this kind of cases, or, by extension, any possible case whose regression model was not a linear one, the study should be designed to account for such change.

Figure 9: Typical allometry in a living organism.



In our opinion, the ideas we have here exposed strength even more the approach known as compositional data analysis. The difficulties encountered by different scholars, and existing in this field are due on the one hand to the need to develop forward this theoretical and methodological corpus, and on the other hand to the need of become confidence with the nature, potential and limitations of the study of these kind of data. In any case, what does not seem to be acceptable is to consider that the problems encountered can be better solved by working with the so called 'standard' approaches, because in those cases that belong to the field of compositional data analysis the 'standard' approaches are just meaningless and wrong, regardless of the effect that this misapplication will induce.

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