

# A compositional approach to stable isotope data analysis

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## Abstract

Isotopic data are currently becoming an important source of information regarding sources, evolution and mixing processes of water in hydrogeologic systems. However, it is not clear how to treat with statistics the geochemical data and the isotopic data together. We propose to introduce the isotopic information as new parts, and apply compositional data analysis with the resulting increased composition. Results are equivalent to downscale the classical isotopic delta variables, because they are already relative (as needed in the compositional framework) and isotopic variations are almost always very small. This methodology is illustrated and tested with the study of the Llobregat River Basin (Barcelona, NE Spain), where it is shown that, though very small, isotopic variations complement geochemical principal components, and help in the better identification of pollution sources.

**Key words:** log-ratio, statistics, isotope, sulphate.

## 1 Introduction: what is an isotope?

Fretwell's Law. "Warning! Stable isotope data may cause severe and contagious stomach upset if taken alone. To prevent upsetting reviewers' stomach and your own, take stable isotope data with a healthy dose of other hydrologic, geologic, and geochemical information. Then, you will find stable isotope data very beneficial." Extracted from: Kendall and Caldwell (1998).

Isotopes of an element contain the same number of protons but different number of neutrons. This difference in the atomic nuclei results on differences in atomic masses. Having too many or too few neutrons creates nuclear instabilities, which limit the existing number of isotopes: there are unstable isotopes (decaying radioactive nuclides) and stable ones (which do not spontaneously disintegrate). In a neutral atom, the number of electrons equals the number of protons. Thus, different isotopes of a given element also have the same number of electrons and the same electronic structure. Because the chemical behaviour of an atom is largely determined by its electronic structure, isotopes exhibit nearly identical chemical behaviour. However, the bond energy is related to the atomic mass, hence heavier isotopes tend to react somewhat more slowly than lighter isotopes, particularly in light elements when mass differences are more contrasted. This is known as fractionation. When fractionation processes occur, the heavier isotope tends to concentrate in the phases with stronger chemical bonds (e.g. SO<sub>4</sub> is preferentially enriched in heavy isotopes whereas H<sub>2</sub>S is relatively richer in light isotopes). Thus, different phases have differences in the isotopic composition. Stable isotopes have several applications in geology and environmental sciences: tracing origin and contribution of sources, determining paleoclimatic characteristics, among others.

Stable isotopes are usually measured as the ratio between the interesting isotope and the most-abundant one, e.g. Deuterium (<sup>2</sup>H=D) against Hydrogen (<sup>1</sup>H). Measuring such a small difference in the number of neutrons cannot be feasibly done in an absolute way, and these ratios are almost always done with respect to international standards. Thus, measures are usually expressed in delta notation,

$$d^{34}\text{S} = \frac{\left(\frac{^{34}\text{S}}{^{32}\text{S}}\right)_{\text{sample}} - \left(\frac{^{34}\text{S}}{^{32}\text{S}}\right)_{\text{std}}}{\left(\frac{^{34}\text{S}}{^{32}\text{S}}\right)_{\text{std}}} \times 1000. \quad (1)$$

since isotopes are actually measured in this way: relative to a standard.

In recent years, the availability of isotope data has increased in several fields, especially since the development of continuous flow analysis techniques. Following Fretwell's Law, isotopic data need to complement an appropriate geochemical and hydrologic characterisation, and statistical techniques are a classical way to obtain such a characterization. Our main goal is therefore to put forward a way to *introduce in the statistical treatment* variables capturing the *information on stable isotope* abundance. We will develop and illustrate our strategy using a case study: a hydrochemical data set from the Llobregat River that contains 14 chemical parameters and 4 isotopic parameters.

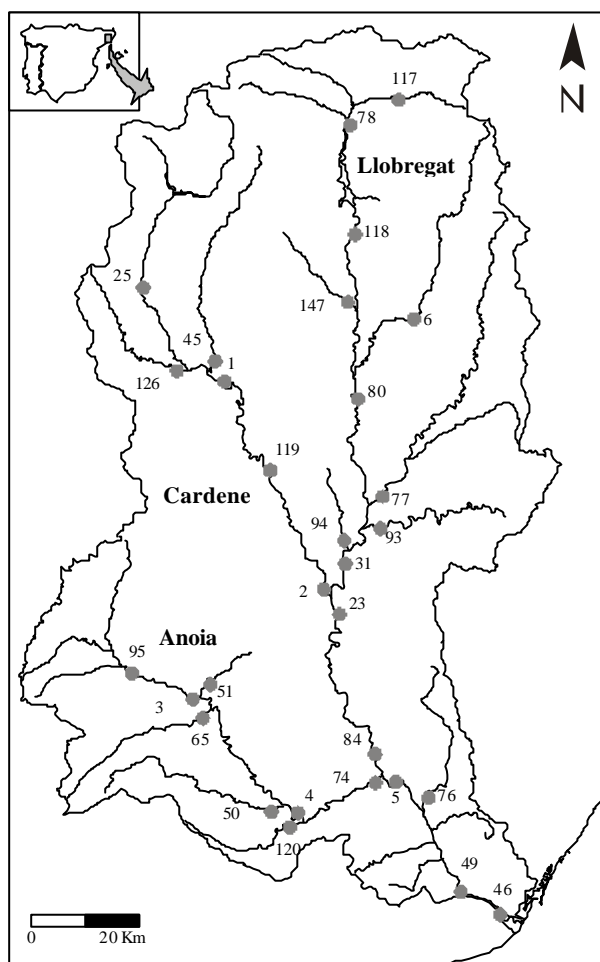


Figure 1. Llobregat River showing sampling sites.

## 2 Case study: the Llobregat River basin

“Gracias a esto, agregó a su *tractatus* un nuevo volumen en el que demostraba de modo irrefutable que el agua de un río nunca pasa dos veces por el mismo punto, salvo en el Llobregat.”

Translation: “Thanks to that, he added to his *tractatus* a new volume, in which he demonstrated in an irrefutable way that no river water flows twice through the same point, except in the Llobregat River”.

Eduardo Mendoza (*Las aventuras del tocador de señoras*).

The Llobregat River is located in NE Spain. It drains an area of 4948.2 Km<sup>2</sup>, and is 156.6 Km long, with two main tributaries, the Cardener and Anoia Rivers (Figure 1). For more information on the River characteristics, see Soler and others (2002), Otero and others (2005a), and Tolosana-Delgado and others (2005). Results of previous work on this area (Soler and others, 2002) show that the weathering of the Tertiary chemical sediments within the drainage basin mainly controls the chemistry of most stream

waters. The major sources of anthropogenic pollution in the basin are identified: potash mine tailing, fertilizers and urban or industrial sewage. They are also chemically and isotopically characterized (Otero and Soler, 2002; Vitòria and others, 2004; and Otero and others, 2005b). In other studies, the coupled use of chemical data with isotopic compositions from strontium (Antich and others, 2000, 2001) and sulphur (Otero and Soler, 2002), allows to quantify, to some extent, the contribution of these sources to water pollution. These previous studies were limited in the time scale, or were focused in small-scale areas.

However, the study was actually conducted during two years at a basin scale, analyzing chemical and isotopic data ( $D_{H_2O}$ ,  $O_{H_2O}$ ,  $S_{SO_4}$ ,  $O_{SO_4}$ , and Sr). Selected chemical parameters were statistically treated and results highlighted two factors defined as equilibrium equations between some of the available components (Otero and others, 2005) thus offering a reduction of dimensionality following the log-contrast approach (Aitchison, 1984). The first factor, considered a geological factor (G), reflects the geochemical signature of the bedrock, enhanced by potash mining. The second factor, taken as anthropogenic (A), is controlled by the relationship between  $NH_4^+$  and  $NO_3^-$ . A detailed analysis of these two factors (Tolosana-Delgado and others, 2005) suggested the existence of three end-members, named W, K, and N, which represent the relative influence of pristine waters, potash mining, and nitrogen pollution sources. This interpretation was grounded on the available analysis of known inputs in the area.

### 3 Methodology: introducing isotopes in compositional data analysis

#### 3.1 Reduction of the data set

Isotope analyses are rather expensive and more tedious than classical geochemical analyses. For this reason, isotopes are not measured for all the individuals. It is normal then to analyse the suite of geochemical variables for the whole sample, and use a sub-sample for the suite of isotopic variables. Then, the first step should be ensuring that the reduction of the sample does not change the statistical results obtained with the geochemical suite.

In our case, the data set used in the statistical treatment of geochemical variables contains 485 measurements. In contrast, oxygen of dissolved sulphate ( $^{18}O$  in  $SO_4^-$ ), and deuterium and oxygen of water ( $^1H$  and  $^{18}O$  in  $H_2O$ ) were measured only in selected samples (approximately quarterly each year) although sulphur isotopes were analyzed in all the samples ( $^{34}S$  in  $SO_4^-$ ). Therefore, the dataset including the isotopic characterisation is reduced to 199 measures. We have compared the conclusions regarding the geochemical suite for these two data sets by means of a biplot (see Otero and others, 2005). Figure 2A shows the biplot of the whole dataset and Figure 2B shows the biplot of the reduced one. Resulting biplots are extremely similar, and minor differences can be attributed to randomness. Consequently, the reduction of the data set will not introduce changes in our results regarding the geochemical suite.

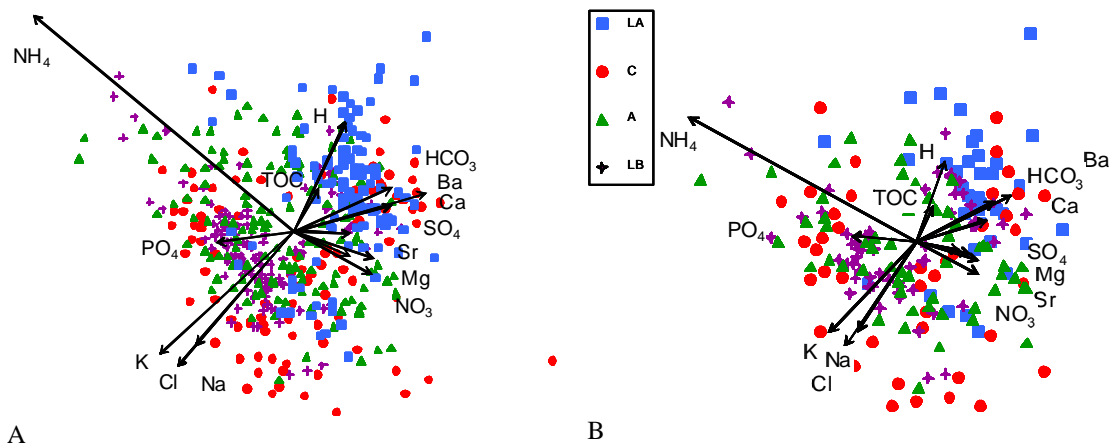
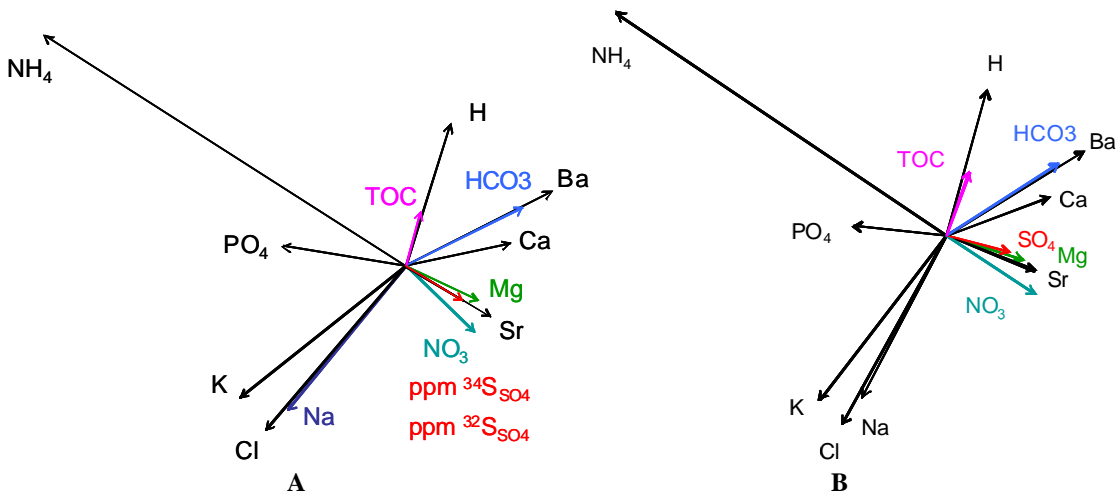


Figure 2. A) Biplot of the whole dataset (57% of explained variance);  
 B) Biplot with the reduced dataset (55% of explained variance).

### 3.2 Working with isotope parts

Isotope data variability is very small compared with variability of chemical data. But if a joint analysis of isotopic and geochemical information is desired (e.g., for discrimination, regression analysis or end-member modelling), these two types of variables must be somehow *pooled* together. Though seldom done, the amount of each isotope as components of the full composition can be easily obtained from the information on relative abundance of the isotopes in the sample and in the standard, when the isotopes was measured in a single chemical species. For instance, in our case sulphur only appear in  $\text{SO}_4^{2-}$ , so using  $\delta^{34}\text{S}$  we can split the amount of sulphate in two:  $\text{SO}_4^{2-}$  with  $^{32}\text{S}$  and  $\text{SO}_4^{2-}$  with  $^{34}\text{S}$ , respectively represented by  $[^{32}\text{SO}_4^{2-}]$  and  $[^{34}\text{SO}_4^{2-}]$ . In this way, our system with 14 chemical variables and an isotopic variable becomes a system with 15 chemical variables. We call this system an *homogeneous* one, because all variables in it are expressed in the same relative scale, and their variations are thus comparable.

Once this homogeneous system is obtained, we could directly do compositional statistics with it. For instance, it is well known that a singular value decomposition (SVD, Eckart and Young, 1936) would give us a series of maximal variant directions as linear combinations of components. In an Aitchison geometry of the simplex, these linear combinations will be weighted products of components, and the graphical representation of the two first dimensions is the compositional biplot (Aitchison, 1997; Aitchison and Greenacre, 2002). Figure 3A contains such a biplot, including isotope data, and Figure 3B contains the biplot without isotope data. The two biplots are nearly identical, and both  $[^{32}\text{SO}_4^{2-}]$  and  $[^{34}\text{SO}_4^{2-}]$  lie exactly in the same arrow thus indicating that differences between them are masked by the variability in sulphate concentration. The biplot with  $[^{18}\text{O}_{\text{SO}_4}]$  and  $[^{16}\text{O}_{\text{SO}_4}]$  is identical to that of Figure 2B. The same results are obtained if water is replaced by  $[^{18}\text{O}_{\text{H}_2\text{O}}]$  and  $[^{16}\text{O}_{\text{H}_2\text{O}}]$ , or [D] and [H].

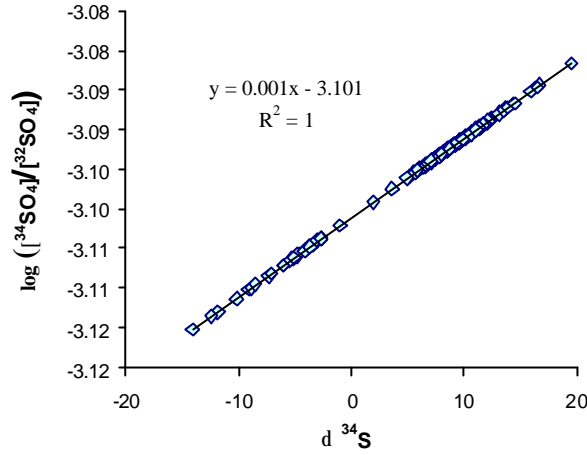


**Figure 3.** A) Biplot (55% expl. var.) of the homogeneous compositional system obtained by splitting  $\text{SO}_4^{2-}$  concentration by the concentration of sulphate with  $^{32}\text{S}$  and with  $^{34}\text{S}$ . Note that these two variables coincide. B) biplot of the original system.

Table 1 (in the appendix) shows the right singular vector matrix of the SVD (containing the loadings of each part on each principal component), for the homogeneous system with sulphur isotopes instead of sulphate. It is evident that no significant change occurred in the biplot, and a comparison of the right singular vectors with those obtained for the original system (Table 2, in the appendix) shows also little or no change, except the new 15<sup>th</sup> non-null column. This column shows us that this last principal direction is

$$\mathbf{h}_{15} \approx 0.707 \ln \left[ \frac{^{34}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}} \right] - 0.707 \ln \left[ \frac{^{32}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}} \right] = 0.707 \ln \left[ \frac{^{34}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}} \right] = \frac{1}{\sqrt{2}} \ln \left[ \frac{^{34}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}} \right], \quad (2)$$

suggesting that the log-ratio  $\ln \left[ \frac{^{34}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}} \right]$  is the adequate way of taking isotope information into account, possibly normalized to unit norm. This singular direction capturing isotopic variation is orthogonal to the rest of the chemical system, due to the standard properties of SVD results. Thus, the inference process in the isotopic direction and the compositional directions may be undertaken independently. Note in passing that (2) is the expression of an immediate ilr coordinate.



**Figure 4.** Scatter plot of the log-ratio of sulphate with  $^{34}\text{S}$  and sulphate with  $^{32}\text{S}$  (ordinate) against the  $\delta^{34}\text{S}$  (abscise), with the equation and the coefficient of determination of the corresponding linear regression.

### 3.3 Relationship between delta notation and log-ratios of isotopes

There is nevertheless a direct relationship between the isotopic log-ratio here derived and the classical delta variable. A Taylor polynomial development of the logarithm function is

$$\ln(x) = \ln(a) + \left(\frac{x-a}{a}\right) - \frac{1}{2}\left(\frac{x-a}{a}\right)^2 + \frac{1}{3}\left(\frac{x-a}{a}\right)^3 - \frac{1}{4}\left(\frac{x-a}{a}\right)^4 + \dots$$

around a point  $a$  (Weisstein, 2005). Taking only the first order of the Taylor polynomial,

$$\ln x = \ln a + \frac{x-a}{a}, \quad (3)$$

and identifying  $x = \left[\frac{^{34}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}}\right]_{\text{sample}}$  in the sample, and  $a = \left[\frac{^{34}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}}\right]_{\text{std}}$  in the standard, we obtain

$$\ln\left(\left[\frac{^{34}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}}\right]_{\text{sample}}\right) = \ln\left(\left[\frac{^{34}\text{SO}_4^{2-}}{^{32}\text{SO}_4^{2-}}\right]_{\text{std}}\right) + \frac{d^{34}\text{S}}{1000}. \quad (4)$$

A regression analysis should confirm then a linear relation like (4). This regression is included in Figure 4, showing a practical determination coefficient of  $R^2=1$ , an estimated slope of 1/1000 and an estimated intercept of -3.101, which is approximately equal to  $\ln\left[\frac{^{34}\text{S}}{^{32}\text{S}}\right]_{\text{std}}$  in the standard.

Summarizing, we have seen that we can split the content of  $\text{SO}_4^{2-}$  distinguishing between the two isotopes of sulphur. The best way to take into account the isotopic information is then through the log-ratio of these two new parts of  $\text{SO}_4^{2-}$ . However, this new log-ratio is proportional to the classical  $\delta^{34}\text{S}$ . Consequently, we can do statistics mixing a composition and an isotopic variable either by splitting the components in isotopes or by including directly a delta variable. If we choose this second option, and want these two kinds of variables to be equally scaled, we will use a definition of  $\delta^{34}\text{S}$  like

$$d^{34}\text{S} = \frac{1}{\sqrt{2}} \frac{\left(\frac{^{34}\text{S}}{^{32}\text{S}}\right)_{\text{sample}} - \left(\frac{^{34}\text{S}}{^{32}\text{S}}\right)_{\text{std}}}{\left(\frac{^{34}\text{S}}{^{32}\text{S}}\right)_{\text{std}}}.$$

Otherwise, we should take into account that the variance and covariances involving the classical  $\delta^{34}\text{S}$  (Eq. 1) are not comparable to those obtained for compositions, and thus variance-covariance matrices will be meaningless.

It is important to note that, though we have here treated only one isotopic variable in a particular case, this methodology is a valid one in general and for all isotopic variables. The linear approximation (3) would not be a valid one if variations in delta were strong. But we know that this is never the case with the usual isotopes. Again, it is important to recall that isotopic variations are several orders of magnitude smaller than geochemical variations.

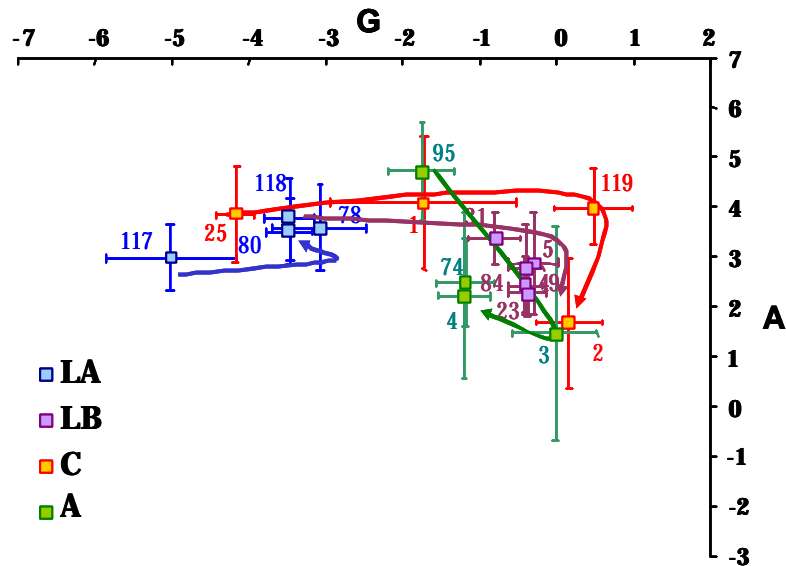


Figure 5. Scatter plot of G factor vs. A factor (see explanation on the text). The arrows indicate the downstream evolution.

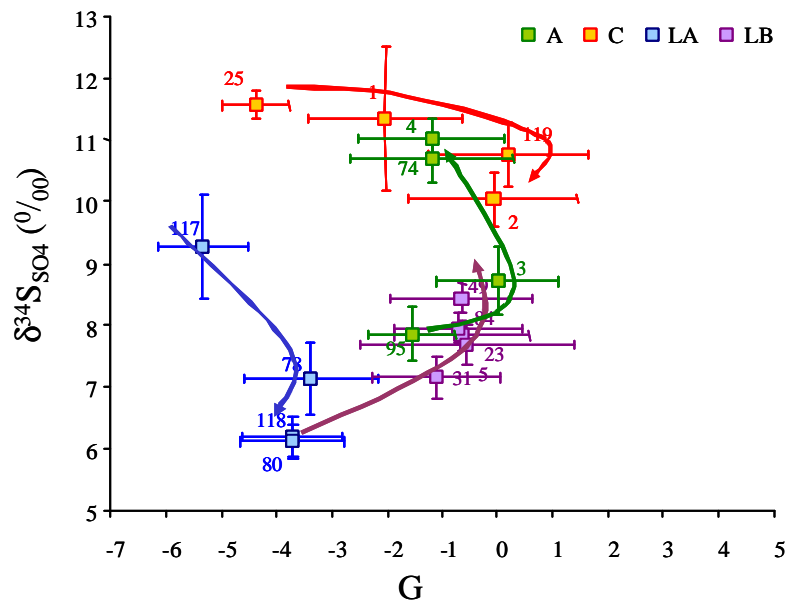


Figure 6. Scatter plot of Factor G vs. the  $\delta^{34}\text{S}_{\text{SO}_4}$ , the arrows indicate the downstream evolution.

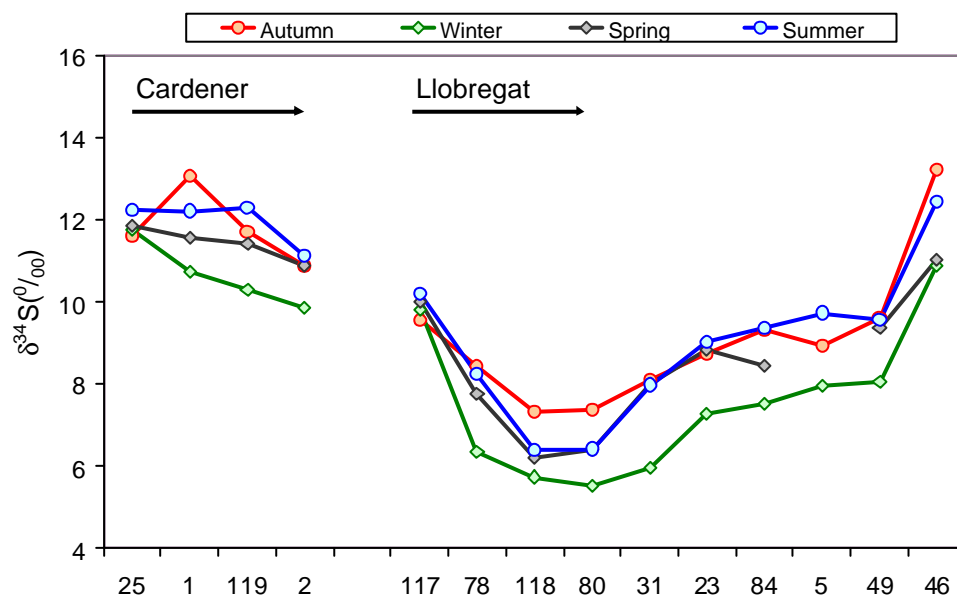
#### 4 Application: sulphur isotopes in the Llobregat River basin.

However, despite this low variability of isotope data, they provide very useful information about the origin of solutes in waters. Because they are rather invariant, isotope data can distinguish between sources of pollution with similar chemical contribution. To illustrate this we can compare the results obtained by the statistical treatment of chemical data, (Otero and others, 2005; Tolosana-Delgado and others, 2005), with isotope data. Figure 5 shows the scatter plot of factor G vs. factor A, where only the main stream of each River is represented. The arrows indicate the downstream evolution. Recalling results of the cited

papers, factor G increases downstream either by the natural weathering of the outcropping materials or by a raise in anthropogenic inputs. The potash mining influence is clearly reflected in an increase in G factor, from sites 1 to 119, and from sites 80 to 31. The interpretation of factor A is not so clear, as it is controlled by the balance between  $\text{NH}_4^+$  and  $\text{NO}_3^-$ . In this case, unpolluted water values are not identified, although urban influence is well detected, e.g. the decrease in factor A from sites 119 to 2, or from sites 95 to 3. To complement this geochemical information, Figure 6 shows the scatter plot of factor G vs. the sulphur isotopic composition of dissolved sulphate ( $\delta^{34}\text{S}_{\text{SO}_4}$ , Eq. 1). As in the previous figure, only the main stream of each River is represented, and the arrows indicate the downstream evolution.

The first point to highlight is that most  $\delta^{34}\text{S}$  values are lower than the expected for the weathering of the outcropping materials. One of the advantages of the isotopic composition, in the studied area, is that the natural values are well identified. The  $\delta^{34}\text{S}$  of the outcropping sulphates ranges from +11‰ to +22‰. Furthermore, the major sources of pollution have been identified and isotopically characterized, e.g. Potash mining lixiviates have a mean value of +19‰; fertilizers have a broader range of values, from 0‰ to +11‰, with a mean value of +5‰. A Power Plant is located in the upper part of the basin, and spills sulphate with low isotopic values to the River (+2.5‰) and urban sewage has a mean value around +9‰.

The second aspect to highlight is the different downstream evolution to the Cardener and the Llobregat Rivers. Chemically (Figure 4), a progressive increase in G factor is observed, and factor A does not show important variations. On the contrary, in the scatter plot of factor G vs.  $\delta^{34}\text{S}$  (Figure 5) a clearly different trend for each River is shown. It is worth noting that the two Rivers have similar anthropogenic inputs, the major land use is agriculture, especially in the upper part of the basin. In both rivers, there is potash-mining activity, and both have an urban contribution, higher in the lower part of the basin. Regarding the  $\delta$ -values, the Cardener River has starting values close to the outcropping sulphates, and has higher values than the Llobregat, indicating a major overall influence of mining effluents (it has also higher values of factor G). The slight variation downstream can be explained by a well-equilibrated balance between potash mining inputs and fertilisers. This is supported by seasonal changes observed in the  $\delta^{34}\text{S}$  (Figure 7), where lower values of  $\delta^{34}\text{S}$  are detected during fertilisation periods (winter). The Llobregat River has lower starting values, influenced by the Power plant emissions in the upper part of the basin. Downstream the low values can be attributed to the input of fertilisers, at sites 78, 118 and 80, and the increase from this site to sites 31 and 23 can be explained by the contribution of potash mining. From that point to the mouth, the major source of sulphate is sewage, and little changes are detected.



**Figure 7.**  $\delta^{34}\text{S}$  down-stream evolution of the Cardener and Llobregat River main stream; mean values for each season are represented.

### 3 Conclusions

We can include the information about the isotopic abundance of a sample relative to the abundance in a standard (the well-known isotopic delta variables) in a compositional framework in two ways. As a first option, if the isotopes take part in a single species, we can split the content of this species distinguishing between the contribution of each isotope. The best way to take then into account this isotopic information is through a log-ratio of the new parts. A Taylor development of these log-ratios shows that they may be taken as proportional to the classical deltas, something confirmed by a regression analysis. This linear relationship offers us the second option: to take the isotopic delta scaled down by  $\frac{1}{1000\sqrt{2}}$ . Such a scaling makes variances and covariances of isotopes and compositional variables to be comparable.

Both options produce nevertheless systems where isotope variances are several orders of magnitude smaller than variance of geochemical parts. However, isotopic information is important because isotopes are closely controlled by a few known processes, which produce very small but strongly meaningful variations. In particular, they are specially used in detecting sources of compounds, mixing processes and the influence of organisms. Consequently, isotope variables are not considered due to their high variability, but due to their high interpretability, as we have seen in the case studied.

Using classical delta notation (possibly scaled down to normalize it with a composition) instead of log-ratios of isotopic species has two main advantages: deltas are directly measured in the lab, and mixing processes produce exactly linear patterns. In contrast, variance-covariance matrices involving a delta variable are meaningless, but correlations keep their use. Log-ratios of parts would nevertheless be a surer option if isotope variations were stronger, something which almost never happens.

### Acknowledgements

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## Appendix: tables of singular value decomposition

Table 1. Right singular vector matrix of the homogeneous compositional system obtained by splitting  $\text{SO}_4^{2-}$  concentration by the concentration of sulphate with  $^{32}\text{S}$  and that of sulphate with  $^{34}\text{S}$ .

	v1	v2	v3	v4	v5	v6	v7	v8	v9	v10	v11	v12	v13	v14	v15
$\text{H}^+$	0.0790	0.3461	-0.0664	0.4960	0.1709	0.6585	0.2280	-0.1212	-0.1622	-0.0562	0.0132	0.0003	0.0364	-0.0224	0.0002
$\text{Na}^+$	-0.2172	-0.3550	0.1389	0.0654	-0.0509	0.1042	0.0810	0.2032	0.0226	-0.1730	-0.1811	0.7809	-0.0546	0.0580	0.0018
$\text{K}^+$	-0.3029	-0.3215	-0.0025	0.4392	0.0515	-0.2661	-0.0208	-0.5307	0.1216	0.4049	0.0286	-0.0651	0.0450	-0.0898	-0.0014
$\text{Mg}^{2+}$	0.1303	-0.0855	0.1795	-0.0710	0.0033	-0.2236	-0.0280	-0.4100	-0.5041	-0.5336	0.1103	-0.0683	0.0325	0.3167	0.0046
$\text{Ca}^{2+}$	0.1921	0.0512	0.0996	-0.0913	-0.0494	0.0497	-0.1722	0.0093	0.3353	0.0155	0.0647	0.0480	0.8378	0.1547	-0.0105
$\text{Sr}^{2+}$	0.1550	-0.1247	0.1652	-0.1698	0.0103	0.1554	-0.1868	-0.1014	0.0282	-0.0362	-0.7948	-0.2626	-0.0740	-0.2531	0.0018
$\text{Ba}^{2+}$	0.2670	0.1798	0.0127	0.2962	-0.0256	-0.3742	-0.1919	0.4480	-0.4718	0.3562	-0.1036	0.0727	0.0471	-0.0044	-0.0010
$\text{NH}_4^-$	-0.6566	0.5596	0.2078	-0.2189	0.2499	-0.1319	-0.1310	0.0468	0.0162	-0.0275	-0.0400	-0.0087	-0.0147	0.0034	-0.0001
$\text{Cl}^-$	-0.2599	-0.4042	0.1284	0.1829	-0.0289	0.1181	-0.0229	0.5089	0.0408	-0.2360	0.2317	-0.5206	-0.0018	-0.0164	-0.0016
$\text{NO}_3^-$	0.1276	-0.1701	-0.5555	-0.2054	0.7134	-0.1144	0.0892	0.0791	0.0522	-0.0450	0.0126	0.0170	-0.0058	0.0022	0.0005
$\text{PO}_4^{3-}$	-0.2281	0.0427	-0.6842	-0.1454	-0.5452	0.1327	-0.2397	-0.0539	-0.1317	-0.0175	-0.0132	-0.0102	0.0001	0.0349	-0.0005
$\text{HCO}_3^-$	0.2162	0.1396	0.0377	0.0079	-0.1104	-0.1699	-0.0627	-0.0617	0.1578	-0.2803	0.3206	0.1324	-0.0936	-0.7671	0.0053
TOC	0.0289	0.1343	-0.0408	-0.0818	-0.2748	-0.2755	0.8284	0.0686	0.1372	0.0112	-0.1672	-0.1251	0.0286	0.0677	-0.0003
$\text{H}_2\text{O}$	0.2653	0.1817	0.0136	0.1885	-0.0615	-0.0931	-0.2498	0.0076	0.5356	-0.0830	0.0279	-0.0037	-0.4751	0.4507	0.0016
$^{34}\text{SO}_4^{2-}$	0.1011	-0.0871	0.1828	-0.3462	-0.0267	0.2163	0.0390	-0.0444	-0.0862	0.3541	0.2455	0.0053	-0.1467	0.0350	0.7068
$^{32}\text{SO}_4^{2-}$	0.1023	-0.0870	0.1832	-0.3464	-0.0260	0.2140	0.0404	-0.0481	-0.0916	0.3465	0.2448	0.0077	-0.1611	0.0297	-0.7073

Table 2. Right singular vector matrix of the original homogeneous compositional system..

	V1	V2	V3	V4	V5	V6	V7	V8	V9	V10	V11	V12	V13	V14
<b>H<sup>+</sup></b>	0.0962	0.3244	-0.0038	0.5826	-0.2127	-0.5781	0.2299	0.1237	0.1703	-0.0298	0.0157	0.0008	0.0324	-0.0251
<b>Na<sup>+</sup></b>	-0.2172	-0.3519	0.1675	0.0097	0.0526	-0.1381	0.0910	-0.1920	0.0021	-0.0945	-0.2284	0.7753	-0.0374	0.0594
<b>K<sup>+</sup></b>	-0.2939	-0.3370	0.0857	0.4076	-0.0700	0.3488	-0.0400	0.5128	-0.1672	0.3374	0.1203	-0.0612	0.0246	-0.0900
<b>Mg<sup>2+</sup></b>	0.1333	-0.0835	0.1875	-0.1760	0.0136	0.1672	-0.0232	0.4198	0.5613	-0.4655	-0.0064	-0.0698	0.0704	0.3097
<b>Ca<sup>2+</sup></b>	0.1965	0.0511	0.0952	-0.1448	0.0601	-0.1074	-0.1626	0.0007	-0.3259	0.0335	0.1573	0.0541	0.8235	0.0855
<b>Sr<sup>2+</sup></b>	0.1550	-0.1185	0.1548	-0.2469	0.0059	-0.2447	-0.1707	0.1185	0.0047	0.2703	-0.6986	-0.2782	-0.0693	-0.2530
<b>Ba<sup>2+</sup></b>	0.2821	0.1599	0.0706	0.2480	0.0183	0.4207	-0.2050	-0.4699	0.4228	0.3684	-0.0034	0.0737	0.0395	-0.0066
<b>NH<sub>4</sub><sup>-</sup></b>	-0.6525	0.5819	0.1422	-0.2473	-0.2353	0.1034	-0.1294	-0.0456	-0.0126	-0.0138	-0.0452	-0.0099	-0.0116	0.0040
<b>Cl<sup>-</sup></b>	-0.2586	-0.4048	0.1767	0.1336	0.0234	-0.1302	-0.0143	-0.5018	-0.0233	-0.2995	0.1592	-0.5178	-0.0040	-0.0160
<b>NO<sub>3</sub><sup>-</sup></b>	0.1376	-0.1959	-0.5603	-0.1889	-0.7039	0.1082	0.0901	-0.0769	-0.0478	-0.0513	-0.0043	0.0167	-0.0041	0.0022
<b>PO<sub>4</sub><sup>3-</sup></b>	-0.2162	0.0184	-0.7069	0.0223	0.5389	-0.1281	-0.2396	0.0519	0.1330	-0.0008	-0.0115	-0.0105	0.0037	0.0346
<b>HCO<sub>3</sub><sup>-</sup></b>	0.2250	0.1320	0.0488	-0.0415	0.1177	0.1417	-0.0594	0.0687	-0.1334	-0.3728	0.2162	0.1365	-0.1673	-0.7542
<b>TOC</b>	0.0365	0.1294	-0.0477	-0.1054	0.2857	0.2537	0.8298	-0.0603	-0.1305	0.0668	-0.1421	-0.1282	0.0400	0.0634
<b>H<sub>2</sub>O</b>	0.2780	0.1664	0.0516	0.1563	0.0565	0.0976	-0.2488	-0.0038	-0.5306	-0.1759	-0.0920	-0.0081	-0.4118	0.4859
<b>SO<sub>4</sub><sup>2-</sup></b>	0.0981	-0.0718	0.1380	-0.4093	0.0492	-0.3145	0.0521	0.0543	0.0771	0.4276	0.5633	0.0265	-0.3288	0.1002