Note: All changes in the manuscript are shown in bold.

Referee #2 – J.J. Egozcue

1. Introduction

To our understanding the article by L. Loosvelt and co-authors is an important contribution (Loosvelt et al., 2012). The authors identify an important problem, the sensitivity analysis to changes in compositional input parameters, and propose a way to deal with. The problem is that input parameters of hydrological models can be compositional, and variations of these parameters should be treated in an appropriate geometry. In the studied case, the input of the model TOPLATS (see references Loosvelt et al. 2012) is the clay-sand-silt composition characterising the soil texture. The goal was to carry out a sensitivity analysis of the output soil hydraulic parameters (SHPs) taking into account the compositional character of the input texture parameters. The presented analysis is methodologically sound and the obtained results are potentially useful for further use of TOPLATS and for improvements in the sampling techniques of soil characteristics. The merit of this contribution is daring to use appropriate compositional techniques despite of not commonly used in this context. Accordingly, the contribution states an important criticism on methods which ignore the compositional character of used data and parameters. We agree with this criticism and we would encourage the revision of methods used in geosciences, and all scientific fields, which deal with compositional data and/or compositional parameters ignoring their character and overlooking the consequences.

At this point, a definition of compositional data or parameters is worth, since the authors use a restrictive definition. However, this view has no further consequences in the paper. They use the classical idea that a composition is a vector with positive components adding to a constant. Accordingly, they are called closed data as it is frequently done in geosciences, e.g. Chayes (1960); Butler (1978); Chayes and Trochimczyk (1978); Buccianti and Rosso (1999). As the authors point out, an important characteristic of compositions is that the only information in a composition is contained in the ratios between the components (Aitchison, 1986). However, compositions are better thought of as equivalence classes of vectors with positive components: two of these vectors are equivalent if their components are proportional (Barceló-Vidal et al., 2001). A further step is that components of compositions do not need to add to a constant (Buccianti and Pawlowsky-Glahn, 2005; Egozcue and Pawlowsky-Glahn, 2011). Typical examples in geosciences are concentrations given in molar concentrations or in mg per liter. This kind of compositions can be changed into (closed) proportions using a perturbation, the addition in the simplex, without loss of information.

In Loosvelt et al. (2012), clay-sand-silt proportions are adequately considered as a composition –see an example in Aitchison (1986)–. However, other compositions are mentioned in the paper. For instance, the soil moisture content _r (m3m□3) can be considered as a two-part composition; also porosity can be treated as a two-part composition. It could have consequences in the sensitivity analysis proposed.

The present comment is centered in three specific points. The first one is related to the fact that the authors avoid the use of ilr-coordinates. The second one refers to some generalization of sensitivity analysis when input parameters are compositional. The third tries to show that the role of the Dirichlet distribution in the sensitivity analysis is irrelevant. These points should be considered as a positive consequence of the Loosvelt et al. (2012) contribution and they are intended to encourage further studies.

2. Use of ilr-coordinates in the simplex

(content see interactive discussion)
The algebra of ilr-transformations allows an easy generalization to more than the M = 3 axes (six points) taken in the perturbation circle presented in Loosvelt et al. (2012).

In a general case where the texture of the soil is described with more than 3 parts, e.g. Parent et al. (2012), the perturbation circle is not easily generalized to the sphere and hyper-spheres. A larger number of points on the hyper-sphere would be necessary and the distribution of the axes may cause difficulties.

- It is true that if the number of perturbation axes *M* or the dimension of the simplex sample space *D* is larger than three (*M>3* and/or *D>3*), the presented methodology based on the operations in the simplex is not easy to generalize. In such case, it is advised to use the roundabout method based on the ilr-transformation and its inverse transformation as suggested by Egozcue. For more complex problems, e.g. *D>3*, it should be further investigated if the presented methodology is practically feasible and how the direction and the number of the perturbation axes should be optimally defined. This study is only a first attempt to perform a

sensitivity analysis on compositional data and as many questions about the generality of the method and the results (see also comments of Reviewer #1) remain there is an incentive for further experiments on this subject.

- The paragraph starting on line 292 (section 2.3.2) is added to discuss the generality of the methodology.

- Lines 209-212 were added (section 2.2.1.) to introduce the role of ilr- coordinate transformation in the context of this paper.

3. Sensitivity, scales and derivatives

A sensible question is, which is the scale of parameter θ or, equivalently, how the difference between two values of θ is computed… A way to deal with the choice of scale of an output parameter θ is to select a one-to-one function φ such that φ(θ) has an absolute scale… The decision on the scale of each parameter is subjective but implications of such a decision should be carefully analysed.

- In this study, the soil moisture content was not considered as a composition but as an absolute value. As such, the calculation of the local sensitivity index was based on an absolute difference between two parameter values. As the reviewer suggests, it would be better to deal with the parameters as compositions and calculate differences based on a perturbation. However, it was chosen to present soil moisture as absolute value in order not to unnecessarily complicate the SA method and to keep it transparent for other users.
- The results of the sensitivity analysis should therefore be interpreted w.r.t. the choice of the scale of the output parameters. Optimizing the formulation of the sensitivity index such that it accounts for ratio scales is an interesting subject for future research.

… Alternatively for D>3, a large number of points on the perturbation hyper-space can be required to compute the scalar sensitivity index. Then, using the gradient in Eq. (2) can simplify the computation of the directional derivatives dramatically.

- This is again a useful remark concerning the generalization of the method towards higher dimensions. The suggested approach is mentioned in the manuscript in an additional paragraph starting on line 337 (Section 2.3.3).
- Lines 529-530 (section 4) are added in the conclusion section to promote the alternative approach using ilr-coordinates when the SA problem becomes more complex than the one presented here (M=3 and D=3).

We would suggest to perform the sensitivity analysis on a (limited) regular grid in ilr-coordinates, where both contour plots of the index and mean values are not distorted. As a traditional way of presenting results, ternary plots may be also useful, but distortion near the borders should be taken into account.

- The reason why a ternary plot has been chosen is because of the traditional way of presenting soil texture. By sticking to the triangle representation and performing all computations on the ternary diagram, we tend to stay close to the soil scientist's view. However, it is true that distortion of the values near the borders may affect the interpretation of the results, but we think that because of a very high sampling density (5000 samples) this effect is minimized.

General comments:

1. *The contribution by Loosvelt et al. (2012) is relevant because it fosters the problem of sensitivity analysis of a numerical model. These kind of analyses are not new, but are frequently overlooked in the standard practice. The novelty is considering the compositional character of the input parameters.*

2. *The sensitivity study of the output hydraulic parameters of the TOPLATS model with the input texture of soil leads to important conclusions. One of them is that USDA-classes seem to be too rough to characterize the soil texture. We would add that three grain classes (silt, sand, clay) are not enough for an accurate description of the soil texture, thus claiming for a revision of the code.*
   - This comment is adopted in lines 479-482 (section 3.2.3.).

3. *Our comments try to point out ways to deal with a more detailed description of the soil texture. Specifically, we remark the importance of working with ilr-coordinates to improve computation, evaluation of mean values of sensitivity indices and plotting techniques.*

Specific comments:

1. *Throughout the paper use baricenter in place of barycenter. We would recommend this substitution.*
   - ok
2. *Powering in the simplex is not commutative, i.e. for a real number α and a composition x, α• x is not x•α. The standard form is α•x. However, this is just a convention, and the authors can use the reverse expression, but a definition is advisable. Note that in standard real operations this is not important as both α and x are real and the implied operation is the commutative real multiplication.*
   - The standard form has been adopted in Eq.(3), in line 260 (section 2.3.2.) and in algorithms (1) and (2).
3. *We do not like to call ξ perturbation factor. In fact, it appears in the form (1+/-ξ), which involves standard addition. We would feel more confortable if (1+/-ξ) were called powering factor or scaling factor (it is a factor in the Aitchison geometry as it is a powering-factor). It is not easy to give an appropriate name to ξ; perhaps something like powering rate thus taking the name of rate from economic terminology: something that has decreased 3% means multiplication-perturbation with the coefficient 0:97.*
4.
   - We deliberately chose not to mention the term perturbation in the context of the basic operations in the simplex (section 2.2.1.) in order to exclusively reserve this term when referring to a variation of a parameter around its base value. The real perturbation operation in the simplex is referred to as vector addition. In the context of a sensitivity analysis, perturbation of a parameter is therefore unambiguous. For that reason we like to preserve the name 'perturbation factor' for ξ. Moreover, the parameter is clearly associated with the sentence "perturbation of x with a factor ξ".

5. *In Figure 2, an ilr-transformation has been used. Although different ilr-transformations consist of a rotation of the figure, we guess that the used ilr-coordinates (balances) were… They should be mentioned in the caption of Fig. 2 (or in the text).*
   - The used ilr-coordinates are mentioned in section 2.3.1 as Eq. (5).
6. *In Eq. (1) summation subindexes do not match.*
   - Ok, corrected
7. *Before Eq. (6), notation yt is used. However, t is only defined after the discussion of Eqs. (6) (7) and (8). A brief description of what is t is therefore convenient before Eq. (6).*
   - The variable *t* is now explained in line 316.
8. *In page 8856, lines 4-6 (before the algorithm listing) the sentence Note that the presented methodology does not allow to calculate the sensitivity for the baricenter as the scalar multiplication p0 _ (1 _ _) has no effect on this composition is wrong. The operation p0 _(1__) is not needed for computation of the sensitivity index, as p0 is a center of a circle and what is powered by 1 _ _ is a (unitary) vector placed at p0. We would recommend to delete this confusing statement.*
   - Ok, sentence removed from the manuscript.
9. *Section 3.2.2, lines 10-13. The statement is unclear, due to the concept of correlation in this context. Which correlation is referred to? A better explanation is advisable.*
   - These lines are reformulated as follows:" In case Cl<35%, the textural sensitivity increases with increasing values of the clay content, whereas in case Cl>70% the textural sensitivity decreases with increasing values of the clay content.".
10. *First paragraph in section 3.2.3 is difficult to read. Please, use short sentences.*
    - ok
11. *Section 3.2.3, lines 28-31. Please, rewrite avoiding repetition of on the other hand and on the contrary.*
    - ok
12. *Section 4, page 8866, line 16. Separate words verythe.*
    - ok
13. *In Reference Egozcue, J. J., Pawlowsky-Glahn, V., Mateu-Figueras, G., and Barcelo-Vidal, (2003) an accent is missing, i.e. Barceló-Vidal.*
    - ok