Estimation of positive sum-to-one constrained zooplankton grazing preferences with the DEnKF: a twin experiment.

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## Answers to Referee 1

The authors wish to thank the referee for his/her helpful and constructive comments.

Experiments attempting to evaluate the robustness of the results to the asymmetry of the spherical transformation have been performed. Some results are highlighted in the answers to referee 2, but we did not include them in the manuscript because they are relatively similar to the results already shown.

Furthermore, we discovered during the reviewing process a work of Nurmela (1995) introducing the hyperspherical coordinate system to remove constraints of sum in geometrical applications (spherical code). A reference to this work has been added in §2.3.

## Main comments

I think that the methodological development would be more understandable by more clearly separating what is general and what is specific. In my view, the most general things in the method are the changes of variables given by Eqs. (3), (4) and (5), transforming the grazing preferences  $\pi_i$  into the new parameters  $\phi_i$ . Such a transformation is the basic idea allowing to apply the ensemble Kalman filter to positive sum- to-one parameters (and maybe also to a broader class of problems, see comment 1 below). Then, the authors make quite specific assumptions about the prior probability distribution for the parameters: (i) the prior probability distribution is specified for the transformed parameters  $\phi_i$ , and the prior uncertainties on the  $\phi_i$  are assumed independent; (ii) the original parameters  $\pi_i$  have equal expected values. Everthing that follows Eq. (6) and all developments in Appendix A depend on these two restrictive assumptions. Then, as an additional parameterization, the authors assume that (iii) the prior probability distribution for each  $\pi_i$  is a triangular distribution [with one free parameter that is tuned so that the condition (ii) is verified]. Eq. (14) and all developments in Appendix B depend on this additional parameterization. To make the paper more understandable, this sequence of assumptions should be made clear to the reader from the very beginning (in section 2.3).

The section 2 has been rewritten in that sense. We hope that is easier to assess how specific the developments are. In a first subsection (§2.3), we present the hyperspherical coordinate system. In a second subsection (§2.4), we suggest several strategies to specify the distribution of the transformed parameters  $(\phi_i)_{i=1:N-1}$ . We have also extended the calculus in order to specify any set of prior expected values and variances for the  $(\pi_i)_{i=1:N}$ .

a In section 2.3, I would present assumptions (i) and (ii) as just one possibility to define the prior probability distribution for the parameters. For instance, it would have been possible to make any kind of assumption for the prior distribution of the original parameters i (e.g. a trunctated Gaussian or any other distribution verifying the constraints), sample this distribution to obtain an ensemble for the  $\pi_i$  and transform the ensemble using the inverse of the transformation in Eq. (5) (which can easily be obtained, see comment 2 below). I understand that, in this way, the joint prior probability distribution for the ?i could not be made perfectly Gaussian (with anamorphosis). But the positiveness and sum-to-one constraints would be verified all the same. Why is it so important that the prior distribution be so perfectly Gaussian, whereas it is never as perfectly verified for the biogeochemical variables? Dont you believe that assumptions (i) and (ii) may be a high price to pay for this?

We agree with the referee. We did not envisage to use the inverse of the transformation to specify the distribution of the transformed parameters  $(\phi_i)_{i=1:N-1}$  because we focus on the specific problem of estimating the zooplankton grazing preferences for which we do not have prior information on their distribution. For that reason, it seemed to us that it was easier to focus on the distribution on the  $(\phi_i)_{i=1:N-1}$  notably to generate samples fulfilling the constraints. However, as suggested by the referee, it is possible to do the inverse when samples of the distribution are available. This point has been added in §2.4 . Furthermore, in order to make the approach less specific, the revised version of the manuscript includes the systems to solve in order to obtain any set of prior expected values and variances for the  $(\pi_i)_{i=1:N}$  and not only

equal expected values. The only assumption that is made concerns the independence of the  $(\phi_i)_{i=1:N-1}$ . However, we do not think that this modeling choice prevent the estimation of the values of the  $(\pi_i)_{i=1:N}$  and we consider that the approach can be useful when no prior information on the distribution of the  $(\pi_i)_{i=1:N}$  is available.

b Since the authors used the assumptions (i) and (ii), I think that the Appendix A can be kept in the paper, but I would urge the authors to simplify and clarify the mathematical developments as much as possible. An alternative would be to remove the appendix, and to derive directly Eq. (14) from the condition (ii) using the transformation (5) and the distribution (13). The only consequence would be that the user would have to redo the computation of the expected value for the i for any other assumption (iii) [which is not necessarily more difficult than computing the characteristic function in Eq. (6)].

As pointed out by the referee, the extension of the system to any set of values  $(m_i)_{i=1:N}$  is straightforward from our previous calculus For that reason, we decided to rewrite the systems in this more general case and the details of the calculus are given in Appendix A.

c The paper would be more understandable if the assumption (iii) [i.e. the paragraph with Eqs. (13) and (14)] was moved at the end of section 2 (as the particular choice that is done in the application). Actually, it is only when I saw Eqs. (13) and (14) that I understood the purpose and the meaning of Eq. (6).

A subsection  $(\S2.4.3)$  illustrating the approach has been added following the subsections describing the systems. We hope it is easier to understand the meaning of these equations.

d Appendix B is not useful and should be removed. The purpose of the appendix is to show that a solution to Eq. (6) [condition (ii)] exist in the particular case of a parametric triangular distribution [condition (iii)]. And the result of the appendix is that a solution exists for less than 3 parameters, which amounts to saying that Eq. (14) [a simple equation without any parameters] does have a solution. I think that this is a very small mathematical detail that should not be published in an oceanography journal.

We agree with the referee that the calculus in Appendix B could be removed. However, the inclusion of new results has led to a change of content of Appendix B which now describes the derivation of the systems required to choose the variances of the parameters  $(\pi)_{i=1:N}$ .

## Other comments

• It would maybe be useful to say somewhere that the method could be easily generalized to variables constrained inside any triangle (in the plane) or any pyramid, using an additional linear transformation.

We agree that the method can be generalized to the constraints:  $\forall i = 1 : N, \pi_i \geq c_i$  and  $\sum_{i=1}^N \pi_i = r$  with  $\sum_{i=1}^N c_i \leq r$  which we expect the reader would find rather trivial. However, we are not sure that this corresponds to the meaning of the remark of the referee. In doubt, we preferred not to include this point in the manuscript.

• It would also be interesting to say somewhere that Eq. (5) is easily (recursively) invertible.

It has been specified in the paragraph  $\S2.4$ .

• The same kind of constraints on the parameters could also be taken into account using a truncated Gaussian assumption, as described in Lauvernet et al. (2009), with the constraints:  $\pi_1 \ge 0$ ,  $\pi_2 \ge 0$ ,  $\pi_3 = 1 - \pi_1 - \pi_2 \ge 0$ . It would be interesting to give the relative advantages of the two methods. I would say: more generality in the inequality constraints in the work of Lauvernet et al. (any set of linear inequality constraints), and more freedom in the specification of the prior probability distribution for the parameters with this method.

We thank the refers for this suggestion. We agree that the parameters  $(\pi_i)_{i=1:N}$  could also be estimated with the truncated Gaussian filter suggested by Lauvernet et al. (2009) under the assumption that they have a truncated Gaussian distribution. However the application of this filter is more complicated than the simple changes of variables described in the manuscript. It requires also the use of a Gibbs sampler in two steps involved in the filter which can be expensive if no simplification can be introduced. The transformation based on the hyperspherical

coordinate system does not allow for any set of linear inequality constraints. However, this problem is slightly out of the scope of the study which focus on positive sum-to-one parameters.

A paragraph introducing the idea has been added in section 2.

• p. 1091, l. 6 - 13: This paragraph is not very clear. Please clarify your statements.

The paragraph has been rewritten (see  $\S2.3$ ). We hope it is clearer now.

• p. 1096, l. 10: I see no reason to mention that Matlab has been used to solve Eq. (14), since it can be solved by elementary root finding methods, and since every-body can easily verify that the values provided are solutions of the equations.

The reference has been removed.

• p. 1097, l. 8: I think that the asymmetry of the transformed parameters is a possible difficulty of the method, in particular regarding the assumption (i) above. A word of caution would be welcome.

We agree with the referee. We performed additional experiments to assess the sensitivity of the estimation to the asymmetry of the transformation. The same previous 20 experiments were rerun with different orders in the transformation relative to the microzooplankton diet. The results are quite similar to the previous ones suggesting that the results present in the manuscript are quite robust to changes in the assignment between the parameters. However, this result could depend on the experimental framework and the use of this approach for another application might require equine additional experiments.

Figures and tables can be found in the responses to the second referee.

• p. 1098, l. 1419: The purpose of the ensemble described here is not obvious. Please reorganize the explanation.

The paragraph has been rewritten. We hope that the description of the experimental framework is clearer now.

• Figs. 3 and 4 are too small to be readable in the printed version of the paper. Please enlarge the fonts or split the figures to make them larger.

We agree with the referee. However, it is mostly due to the landscape format used for the manuscripts in OSD. Both figures are meant to fit the portrait format used for the OS articles. We did not assume that the rotation of the format would lead to such a reduction of the size of the figures. However, we think that both figures are more easily readable in the OS portrait format.