

## ***Interactive comment on “Technical Note: Improved Sampling of Behavioral Subsurface Flow Model Parameters Using Active Subspaces” by Daniel Erdal and Olaf A. Cirpka***

**Anonymous Referee #2**

Received and published: 12 May 2020

The current work presents a sampling strategy for those cases when some values of the investigated model output(s) are classified as unfeasible/unacceptable and the corresponding parameters sets are labelled as non-behavioral.

A key step is the transformation from the original  $N$ -parameters space into the space spanned by the  $n$ -most relevant eigenvectors (here two are considered, i.e.,  $n = 2$ ). Then, in this reduced dimensional space an active region is identified (i.e., the active subspace) is identified (see Fig. 2 where all the space above the red line is the active subspace). Then a set of parameters is chosen to be behavioral or not (i.e., the associated output(s) belongs to the active subspace or not) in a two stages approach:

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(1) a surrogate model of dimension  $n$  in the space spanned by the  $n$ -most influential eigenvector is built and then used to check if a parameter set is behavioral or not, as a ‘first approximation’; (2) if a parameters set passes stage-1 the full model is run for that parameters set a second check on being or not behavioral is done. Then only stage-2 parameter sets are retained for successive analysis. The main gains here are due to the reduction of the dimension (from  $N$  to  $n$ ) and the use of a surrogate model in the  $n$ -dimensional space to skim those parameters sets that are not behavioral.

The improvement/modifications proposed in the current work are during stage-1, where an additional constrain is added: a parameters set passes stage-1, if in its neighborhood there is a certain fraction  $P$  of parameter sets that have already passed stage-2.

The paper is of interest and well written. There are some unclear (at least to me) points which I would like to be addressed before publication, hoping for a more clear and more accessible work after revision.

Comment 1 In both approaches, after 100 parameters sets passed stage-1 the eigenvector decomposition is re-done, and so the surrogate in the  $n$ -space dimensions is built again. My understanding is that the output(s) values associated with these 100 samples are obtained through the  $n$ -dimensional surrogate model (before adding the 100 samples), right? If this is the case, isn't there the risk of ‘guiding’/‘move’/‘bias’ the active subspace toward the results of the surrogate model? For example, in Fig. 2 the new extra 100 stage-1 accepted points will all falls along the purple curve (along its branch above the red line). This could be an issue if the surrogate is doing a poor job. Am I wrong?

Why not use stage-2 accepted sample (even though they require full model runs) to update the eigenvectors/eigenvalues? This will avoid the issues associated with a possibly poor surrogate modelling.

Comment 2 How is the algorithm initialized? Which is the size of the sample to build the first  $n$ -dimensional subspace? How is relevant? For example, in Fig. 2 there are

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previously analyzed parameters samples/output, they should come from a set of full model runs (then they are updated after 100-samples pass stage-1t, see the previous comment).

Comment 3 Acceptance ratio: this the ratio between the stage-2 accepted sample and the drawn samples, right?

Why is it a function of the stage-2 accepted samples (see Fig. 3)? I don't see this aspect being used in the algorithm (both previous and current versions) at any step. I would have expected a dependence on the stage-1 accepted samples.

Moreover, as  $P$  (i.e., the fractions of neighborhood accepted, at least at stage-1, samples) increases I would expect lower acceptance ratios, i.e., it becomes harder for a sample set to be accepted as a larger fraction of its neighbors have to be in the active subspace (i.e.,  $P$  increases). (see also lines 116-117 that go along this line of reasoning). Please clarify.

Isn't that, since  $P$  is the exact fraction (not an exceedance fraction) of good neighbors, as  $P$  increases the active subspace is updated (on top of 100 samples that pass stage-1) by favoring those regions of the active subspace that are the most distant from the threshold condition (e.g., upper left part of Fig. 3a) where it is more easy to have  $P$  high than low? Then, the  $n$ -dimensional surrogate will be update by favoring these far-from threshold condition regions leading to a poor behavior (due to its global character) in those regions close to the threshold conditions (e.g., lower right region in Fig. 3). This is then reflected in the decreased quality of the behavioral parameters pdfs as shown in Fig. 4. Or maybe, I am just speculating too much here. It could be of interest to see how the  $n$ -dimensional surrogates evolve as a function of  $P$ , for example after some updates are conducted to see if there is this tendency or not.

Comment 5 Since a surrogate model is used to mimic also the full model response (see Sec. 2.2) I would suggest to refer to this as 'full-model-surrogate' in order to mark the distinction with the surrogate model build in the  $n$ -dimensional space.

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Interactive comment on Hydrol. Earth Syst. Sci. Discuss., <https://doi.org/10.5194/hess-2019-629>, 2020.

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