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Interactive comment

Interactive comment on "Fast sensitivity analysis methods for computationally expensive models with multidimensional output" *by* Edmund Ryan et al.

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Reviewer's comment #1: The PCA which brings the most novelty and potentials should be developed.

Author's response #1: Thank-you for this comment. I will include further details in the discussion about the PCA method. Changes to be made in manuscript: Further details to be included in the discussion in order to elaborate more on the PCA method.

Reviewer's comment #2: page 9: the authors should precise X are inputs and Y outputs in Eq (1) as well as their dimension in the context.



Discussion paper



Author's response #2: Thank-you for spotting this omission. I will include these details in the revision. Changes to be made in manuscript: I will define X and Y following equation (1) and also define what E() and var(Y) mean.

Reviewer's comment #3: page 9: "the method operates by ïňĄrst generating N*2p matrix ..." this ïňĄrst step of the method is not clear for unfamiliar readers

Author's response #3: Good point. I will explain what I mean. Changes to be made in manuscript: I will clarify that I mean a matrix with N rows and 2p columns. I will also be clearer about what I mean by samples.

Reviewer's comment #4: page 13: the difference the GP and the GAM methods should be clariiňAed

Author's response #4: A fair point. I will make the point that with the GP emulator, it is the emulator + eFAST to get the SIs, but with the GAM we can compute the SIs directly with no emulator. Changes to be made in manuscript: In the text on page 13, I will make it clearer about how we're using the GAM to estimate the sensitivity indices as stated above.

Reviewer's comment #5: page 14: the authors say that the p inputs x are independent variables, the independence is an assumption required to apply the proposed method. To extent this hypothesis is realistic? The authors could have precised this assumption earlier in the text to my opinion

Author's response #5: I do not understand your question. However, in response to your second sentence this is a fair point. I will make it clearer earlier in the methods that the inputs are assumed to be independent. Changes to be made in manuscript: Following equation (1), I will add detail to make it clear that the decomposition of the variance of the outputs into its main and interactive effects is done under the assumption of the inputs being independent.

Reviewer's comment #6: page 15: further details should be given on how the sensi-

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tivities with the hybrid methods. Moreover, one beneïňĄt of using PCA in more general setups is to work with independent variables (PCs). Could the authors justify the threshold of 99% in the PCs selection? This seems a high value compared to some common use of PCA

Author's response #6: Yes, I agree with the first point. I realised that my description of the PCA approach, I did not explain how the multi-dimensional model output is reconstructed from the PCAs, and thus how the sensitivity indices are computed. I will add this detail in. The 99% threshold seems valid for this study at least. If you look at figure 2d, you can see that even with 99% of the variance of the model output explained, the median absolute different between the emulator versus chemistry model outputs from the validation runs is okay but could be better. Setting the PCA threshold lower (e.g. 95%) may be sufficient for other studies but for this study it would resulted in a poorer performance by the emulator (i.e. it would have resulted in a lower R² value and a higher MAD value in figure 2d). Changes to be made in manuscript: I will add detail to the PCA part of the methods section to make sure that it is completely clear how the method works and how the sensitivity indices are computed. I will also add a sentence to defend the threshold of 99% for this study, but also explain that lower thresholds may be okay for different modelling setups.

Reviewer's comment #7: How do the authors determine the number of needed runs from the emulators in this study.

Author's response #7: The rule of thumb is 10 * p where p = no. of input factors. Changes to be made in manuscript: I will include this detail and a reference to back it up in the 'Experimental Setup' part of the methods.

GMDD

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