26/12/2021

We thank the reviewers for the time and expertise they have invested in these reviews. We'll reply to individual points below, and we remain at your disposal for further explanations concerning our answers if needed.

Reference report on "RKHSMetaMod: An R package to estimate the Hoeffding decomposition of a complex model by solving RKHS ridge group sparse optimization problem"

This revised version addresses most of my previous comments. I have following minor comments, mostly of which can be easily addressed by the authors. Some comments are for further discussion within the authors' research group for future projects.

1. Minor comments

- 1. I like the review of « related existing statistical packages to RKHSMetaMod ». However, these paragraphs and some technical discussion in introduction may be shortened or moved to Appendix/supplementary materials.

We have reviewed « related existing statistical packages to RKHSMetaMod ». In order to shortened this part of the introduction, we have removed some of the references and preserved those that are more relevant to the rest of the document.

- 2. The subsection « RKHS construction » on page 7 may be put in the Appendix as it may be good to introduce the package with minimum distraction from the theory. After Equ. (7), it may be good to specify that the RKHS norm $\|.\|_{\mathscr{H}}$ and RKHS space will be defined in the Appendix.

Done, we thank the reviewer for the suggestion.

- 3. Equation (11) is interesting. This seems to be a penalty by RKHS norm and empirical L_2-norm. The mixed use of two penalty (L_2-norm and RKHS norm) was shown to be equivalent to the « scaled Gaussian process » for model calibration/inverse problem in [2] and [3] (see e.g. equation (12) in [3]). The authors do NOT need to cite these work, as they are developed for model calibration. I mention them here to initiate some discussion within authors' group about the connection. Some derivation (such as the construction of the processes that lead to these two norms, marginalization of latent processes for computation, etc) in these papers may be helpful for future development of authors' approaches.

We thank the reviewer for the suggestion.

- 4. Are the $\|.\|_n$ in Equ. (11) and $\|.\|$ in Equations after equation (13) the same as both of them are Euclidean norm for variables in $\mathbb{R}^n$?

Not exactly: we have $\|.\|_n = \frac{1}{\sqrt{n}}\|.\|$. For example let X be a vector of n components $X_1, \ldots, X_n$. The empirical L_2-norm of X is $\|X\|_n = \frac{1}{\sqrt{n}}\sqrt{\sum_{i=1}^{n} X_i^2}$. We use the notation $\|.\|$ to show the Euclidean norm (called also L_2-norm) of X : $\|X\| = \|X\|_2 = \sqrt{\sum_{i=1}^{n} X_i^2}$.

- 5. Table 1 on page 9, it may be good to implement the kernel with Matérn 5/2 as this is typically adequately smooth (since the sample path is twice differentiable). Matérn 5/2 is the default kernel in e.g. DiceKriging and RobustGaSP packages.

We agree. We intend to add this kernel in the future version of the package on CRAN.

- 6. Page 9 point 2, « The RKHS meta-model with at most qmax active groups ». Here is each active group an element $v \in \mathscr{P}$? It is not quite clear to me what the group in means here.

We realize that this part of our explanation in the paper is perhaps not clear enough. By active groups we mean the groups $v \in \mathscr{P}$ that are not zero and constitute then the support $S_{\hat{f}}$ of the obtained meta-model $\hat{f}$. The RKHS meta-model with at most $qmax$ active groups has then at most $qmax$ groups in its support, i.e. $|S_{\hat{f}}| \leq qmax$. We modified this sentence in the paper.

- 7. The algorithm 1 and 2 seem to directly truncate the small coefficients to be zero, which may be different than the group lasso algorithm in [1]. Maybe this is due to the lack of closed form expressions in iterations, but then it may let readers wonder whether the sparsity comes from penalty in the model or from truncation in algorithms.

It appears that there is a misunderstanding. In these algorithms the small coefficients are not truncated to be zero, instead we have the necessary and sufficient conditions for θ to be a solution to the expressions $C_{g,v}$ (for algorithm 1) and C_v (for algorithm 2). This part is presented in [1] as Proposition 1 (equations (2.2) and (2.3)), and in our paper in Sections « RKHS group lasso algorithm » and « RKHS ridge group sparse algorithm » (Case1 and Case 2) of the Appendix (supplementary materials).

- 8. On page 23, the function in example 3 is very smooth so Matérn 3/2 is probably not going to work well as the sample path of the process is only once differentiable. Matérn 5/2 are often used instead for these smooth functions. This is just a comment so authors may not need to change if Matérn 5/2 was not implemented in the authors' package yet. Overall I like the added numerical comparison.

We understand the reviewer's point of view. We used the Metérn 3/2 kernel because in the current version of the **RKHSMetaMod** package we have not yet implemented Matérn 5/2 kernel. We agree with the reviewer and intend to add this kernel in the

future version of the package on CRAN. However, this example has already been addressed in Gu et al. (2019) where they use kernel Matérn 5/2, and the obtained GP based meta-models by the **RobustGaSP** and the **DiceKriging** packages do not differ much from those obtained using Matérn 3/2 (please see Figure 4 of our paper and Figure 6 of Gu et al. (2019)).

- 9. Please throughly check the language problems and reduce repeated messages. Here are a few examples:

We have done the paper revision several times and « removed » the language problems.

- Page 4, « In particular we can mention the implementation of Kriging based global sensitivity analysis » may be changed to « In particular, Kriging method can be used to reduce the number of observations in global sensitivity analysis. »

Done, we thank the reviewer for the correction.

- Example 3 on page 19, the « A time saving trick… » seems to be informal.

We agree, we changed this part of the title to « A time-efficient strategy …».

- « the the » appear on page 18 and the caption of Figure 4.

Done, we thank the reviewer for the correction.

- 10. The format in the reference are not very consistent. E.g. the conference was spelled as « Advances in Neural Information Processing Systems » somewhere and « NIPS » elsewhere. In « A correspondence between bayesian estimation on stochastic processes and smoothing by splines », the first letter in *Bayesian* should be capitalized.

We thank the reviewer for the corrections. We have made a complete revision of the references.

- I consider this article to be publishable after the authors address these issues.

Content of the editor's email '[RJournal 2020-165] journal submission'

- The paper would benefit from being shortened considerably. The referee makes some suggestions. In addition, it is not necessary to duplicate function documentation in the paper.

We applied the referee's suggestions. We understand the reviewer's point of view about the function documentation and moved it to the supplementary materials. We suppose that this documentation is useful since it contains much more details about the functions parameters (and algorithms used in these functions) and allows the reader to make links between paper notations/formulas and the functions parameters/arguments.

- I recommend you move some examples to the package vignette. The package itself would benefit from a vignette as this is what will attract users. Alternatively, move some examples to supplementary materials.

We thank the reviewer for the recommendation. We agree and intend to provide vignette in the future version of the package on CRAN. However, we decided to remove « Estimate the meta-models with at most "qmax" active groups » in the paper, as an example very similar to this one (with smaller number of observations and different parameters) has already been studied in the package documentation on CRAN.

- The Appendix should also be part of the supplementary materials. For published papers, the R Journal distributes these materials along with your paper.

We moved the Appendix to the supplementary materials.

- Please do not put CRAN links in the paper. Use the R function citation to generate references.

We replaced CRAN links in the paper by R function citations.

By applying the reviewers recommendations, the length of the article is considerably reduced (23 pages for the original article + 12 pages for the additional material). We hope that the size of this new version of the article is within the range of standard R Journal articles. If this is not the case, we remain at your disposal for further recommendations regarding the length of the article.

References

- M. Gu, J. Palomo, and O. Berger, James. RobustGaSP: Robust Gaussian Stochastic Process emulation in R. The R Journal, 11(1):112, 2019. ISSN 2073-4859. doi: 10.32614/rj-2019-011. URL http: //dx.doi.org/10.32614/rj-2019-011.