

## ***Interactive comment on* “The design, deployment and testing of Kriging models in GEOframe” by Marialaura Bancheri et al.**

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R1: The technical paper presents a package for the interpolation of climatological variables using kriging techniques. The structure of the package is described, and the results of the application to two datasets (a rainfall and a temperature one) are presented. The authors also provide a comparison with the R package gstat. The technical paper aims at describing a package that could be of interest for the geoscientific community due to the fact that it is specifically designed for the interpolation of climatological variables and is suitable to be easily merged into hydrological models. The manuscript then would fit the purposes of the journal, if focused on the description of this package. Despite this, the aim of the paper is not clear. On the one hand, reading the abstract, the expected focus is the tool itself: its capability and the novelty it intro-

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duces in comparison with the available software. On the other hand, going through the paper one can realize that just a limited part of the work is focused on the package, and the core of it is focused on the analysis of the results obtained with the different tested kriging methods. Considering that a wide geostatistical literature focused on the assessment of the quality of the interpolation of climatological variables already exists (e.g., Hartkamp et al., 1999, Moral F. J., 2010, etc.), and that the analysis of the performance of the package are limited to sect.6, I think that the authors should adjust the focus of the whole manuscript (or at least clarify their aims) before it can be accepted for publication.

A1: The authors thank the reviewer for her/his observations, which helped us improve our manuscript. This response does not yet produce a new manuscript, which will be submitted after the closure of the review phase, upon request of the Editor. We introduce here, however, the main adjustments that we will make in the final version of the revised paper based upon the reviewer's suggestions. According to the suggested reviews, we will try to focus more on the package and on its core and shorten the analysis of the results. According to what is stated in the abstract, we will try to respect the purpose of the study, which are: (1) to present a geostatistical software easy to use and easy to plug-in to a hydrological model, (2) to show a practical example of an accurately designed software in the perspective of reproducible research, (3) to show the goodness of the software applications, in order to have a reliable alternative to other traditionally used tools. Moreover, we will try to make a better comparison between SIK and other available software, especially with R gstat.

R2: A series of major comments follows, all related to this topic, and some minors ones are added, that I think the authors should address before the manuscript is ready for publication. Major comments Most of the manuscript is dedicated to the kriging methodology. The use of kriging methodologies is quite established in the hydrological literature and many studies on the performance of the different kriging methods can be found. The core part of the paper should be the description of the tool and the

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assessment of its potentialities.

A2: According to the reviewer suggestion, we decided to move all the equations related to the Kriging theory to the Appendix A and to leave in the text only the most important references. In this way, the core of the paper is going to be the section of the design of the package and the assessment of its potentialities.

R: In the detail:

1. My opinion is that the authors dedicate too much space at the description of the theoretical basis of the kriging (Sect. 2) while some references and a general outline would be enough.

A1. As stated in the previous answer, we moved all the equations of section 2 to a related appendix, leaving only few references in the main text.

2. The analysis of the results of the case study turns out to be the core of the paper (Sect. 5 is the longest one with 6 out of 12 figures dedicated). Section 5 should be revised, shortened, and the number of related figures should be reduced. The interest of the case study is in checking the functionality of the package rather than to carry out an analysis of the performances of the various interpolators

A2. According to the reviewer suggestions, we decided to modify the figures, in order to present only three figures for each case (temperature and rainfall): the fitting of the experimental semivariogram, the leave-one-out results using a single semivariogram model and the raster interpolation, using a single semivariogram model, overlapped to the bubble plot of the errors. For example, Figure 6 now shows only the comparison of the interpolations between the 4 types of Kriging, using the Bessel semivariogram model.

3. While the structure of the tool is clearly explained in sect. 3 the analysis of the performance, compared to other software, is not sufficient. As the authors themselves state, it is an important point “to justify the introduction of an alternative software”.

The authors just refer to general “way longer” (L.5 P.19) computational time of gstat compared to SIK, and a comparison of the NSE for a single model (figure 12). This does not appear enough for a scientific paper: the authors should provide numbers and figures to support and highlight performances of their package in comparison with other software. Their opinion of “greater ease” (L.8 P.19) is not enough, considering that gstat turns out to be more versatile under some points of view (e.g., it considers both omnidirectional and directional variograms) and that there are some other kriging packages offering a user-friendly and easy-to-manage interface (e.g., the v.kriging command in GRASS-Gis).

A3. We agree that previous analysis could appear not too much accurate for a scientific paper. However, a quantitative comparison of the two tools could be unfair (for gstat, at the end). SIK and gstat have different objectives indeed. The software gstat is suitable for use in simple tasks with short scripts, because of its C computational core, embedded in R which is flexible and easy to use. It is, instead, hard to plug-in to a hydrological model, which involves temporal and spatial steps (because R coded for-loops are really slow, being an interpreted language). Besides implementing modelling solutions (MS) which mix for instance Java and R is possible (for instance our new version of the OMS console can do it - at scripting level) but it cannot be considered a clean solution for building an operational tool (R binding into OMS was mostly intended to be used in the analysis of results, more than in computing them). SIK, instead is suitable to fit into large and complicated modeling solution because it is fully OMS-compliant and because of the JVM performance optimizations that comes in when the same algorithm is executed several times (like the kriging interpolation for a year of hourly time steps). However, we changed the text adding more information about differences and similarities between the two softwares. Moreover, we modified the plot related to the temperature comparison (there was also mistake) and we added a new plot on rainfall interpolation, with further information about the comparison. The following part was added to the text of the new manuscript: “A comparison between SIK and the R package `gstat` was made in order to highlight their differences and

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similarities, and to justify the deployment of an alternative software. Benchmarks or quantitative performance comparisons would not have been useful or completely truthful since the "velocity" of computation (a classic quantitative comparison) depends on too many factors, some of which are described below. Therefore, we performed a qualitative comparison between the two softwares accounting for design, the implemented features, and the accuracy of the results. In our opinion, the two tools that we analyzed have different purposes. This can be seen just by looking at the features of the relative programming languages. The gstat software is developed in C with a part of the code in R language. It must be executed using the various R environments. SIK is developed in Java (7) as a group of OMS components and it can be executed form within the OMS console, as a stand-alone Java programs, or embedded in other codes in languages that support Java bindings. Java is slower than 3rd generation languages such as C. However, in the course of Java development several optimizations, such as "just-in-time compilation" and "adaptive optimization", have been introduced to improve the performance of its Java Virtual Machine (JVM). These techniques identify recurrently executed algorithms, so called "hot spots", and dynamically recompile them at run-time. Eventually, the hot spots gain valuable computational speed. C is one of the fastest compiled languages. But only the computational core of gsta\$ is coded in C; the management of temporal steps, such as "for-loops", and data structures must be scripted in R. Undoubtedly, R is a very powerful programming language, mainly because of its flat learning curve, and easy syntax and semantics, but it is fully interpreted, which makes it very slow. As a result, the comparison of the speed of computation for a single temporal Kriging interpolation is unfair against Java, since the JVM cannot exploit its optimization tools for a single computation. On the other hand, the comparison of the speed of computation for a year of hourly Kriging interpolations is biased against R, because temporal steps affect most of the computational time. In terms of functionality, gstat computes both omnidirectional and directional semivariograms, while SIK does not implement directional semivariograms yet (although we have included this feature on the software wish list). Furthermore, gstat provides four more

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theoretical semivariogram models with respect to SIK, these are: Matern, Matern with Stein's parameterizations, Wave, and Legendre. Adding the desired theoretical model to any SIK-TV component would be easy and straightforward, thanks to the DP implemented, as shown in Figure 2, but they are not available at present. Regarding the estimates that the two packages offer, these are usually different. Comparisons were made with both the temperature and rainfall datasets used in section Setup. Semivariograms were computed using the same number of bins and cutoff distance. Figure 12 shows the results of the temperature interpolations done with SIK and gstat, in terms of NSE, RMSE, PBIAS and  $R^2$ : the overall performances of both tools are very good. The NSE values are always above the 0.65, while the RMSE are always lower than  $2^\circ\text{C}$ . Figure 13 shows the results of the precipitation interpolation done with SIK and gstat, in terms of NSE, RMSE, PBIAS,  $R^2$  and cumulative volumes. Also in this case, both softwares are able to reproduce the rainfall event well, simulating the peaks. The results obtained for station ID 1152 are very good for both softwares, with a  $\text{NSE} > 0.9$ . Both softwares show slightly worse results for station ID 2170, with lower values of NSE and  $R^2$ , higher RMSE, and an overestimation of the total rainfall (19 mm with gstat and 20 mm with SIK, compared to the 16 mm recorded by the gauges). In conclusion, gstat is a powerful, flexible tool to get fast results with fast scripting in answer to single, specific questions (with some implementation efforts user-side); SIK is a tool that is ready to be integrated into broader MS, specifically because of its OMS-compliant design. The interpolations of both temperature and rainfall confirm the quality and accuracy of the predictions obtained using the SIK package, demonstrating that it is a good competitor of R gstat."

R: Minor comments 4. Abstract: the abstract should be reviewed according to the modification of the structure of the paper. At the moment it does not describe the focus of the work.

A4. We revised the structure of the paper, trying to follow the three purposes stated in the abstract, according to the reviewer suggestions.

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5. L.9, P.2 – It must be pointed out that GRASS-GIS is also available as an open-source GIS offering a user-friendly (*v.kriging*) function for performing kriging

A5. In the Introduction chapter, according also to the reviews of the Referee #1, we added some missing software that was worth mentioning, among which GRASS-GIS. Now a better comparison of SIK with the existing open-source software is present. The following part was added to the main text: “Several geostatistical tools are made available to the scientific community. Among them, PyKrige (<https://github.com/bsmurphy/PyKrige>), SAGA GIS kriging ([www.saga-gis.org](http://www.saga-gis.org)), GRASS ([grass.osgeo.org](http://grass.osgeo.org)), Surfpack (<https://dakota.sandia.gov/content/surfpack>), R gstat ([www.cran.r-project.org](http://www.cran.r-project.org)) and the High Performance Geostatistics Library HPGL (<https://www.github.com/hppl>). However, only few of them could be considered as alternatives of SIK, i.e. the ones that are open source, comprehensively documented and actively developed: – Dakota (Surfpack): C++ software with flexible interface that provides optimization algorithms, uncertainty quantification, parameter estimation, and sensitivity analysis for supporting computational models and simulators (Adams et al., 2009); – PyKrige: python package that allows for both 2D and 3D ordinary and universal Kriging computation with flexible design for custom variogram implementation (Murphy, 2014); – gstat: R package (computational core coded in C) that supports block kriging, simple, ordinary and universal (co)kriging and many other features (Pebesma, 2004), (Gräler et al., 2016). It is historically the leading software in this field. While GIS-based tools, such as QGIS and GRASS (*v.kriging*) Krings, are easily included into scripts leveraging GIS capabilities, they are not easily included into complicated MS. As well as being open-source, SIK is the only Java-based and component-based software of those mentioned above. Moreover, it implements a quick way to plug-in to hydrological models and automatic calibration algorithms. We decided to compare the performances of SIK and R gstat, since the latter is one of the most widely used tools in the scientific community.”

6. Variables should be named always in italic (e.g., “*B*” L.22, P.3), and measurement

units not in italic (e.g., km<sup>2</sup> L.1, P.9)

A6. Changed accordingly

7. Figure 1 and 2 can be merged together as they differ only for the last block. 8.

A7. Figure 1 was changed accordingly.

8. APPENDICES: I think the authors make a misuse of the appendices. Appendix A could be merged in the main part of the paper as deal with an important phase of the development of the package and Appendix D is almost useless for the aims of the paper (the table should be provided as supplementary material). Reducing the number of the symbols also Appendix B would be useless, and the meaning of the symbol could be inserted along the main text.

A8. All the Appendices were revised according to the reviewer's suggestions. In particular: - Appendix A now introduces the Kriging equations; - Appendix B contains the list of Acronyms; - Appendix C contains the description of the GOFs; - Appendix D contains the list of semivariograms models implemented in SIK.

9. Writing style and use of English could be improved: the manuscript would benefit from extensive English editing by a native speaker. The text should also be double-checked for typos and other minor errors (a non-exhaustive list follows): o L.18, P.1. "anong" -> "among" o L. 8, P.2.

A9. The English is going to be improved in the revisions and also the spelling errors.

10. There is a useless open bracket o L. 4, P. 4.

A10. Changed accordingly

11. "Appendix A" -> "Appendix C" o L. 17, P. 5

A11. Changed accordingly

12. I don't think "contemporary" is a proper word in this case o L. 10, P. 8



A12. Changed accordingly

13. “classes” -> “class” o L. 14, P. 8

A13. Changed accordingly

14. “ . . . in D” -> “..in Appendix D” o L. 7, P. 10

A14. Changed accordingly

15. “where” -> “were” 10.

A15. Changed accordingly

16. Reference style is not uniform, sometimes brackets include only the year (e.g., L.1, P.2) and sometimes name and year (e.g., L.25, P.2).

A16. We will try to check all the reference styles.

17. Please adopt the journal style.

A17. We will adopt the journal style.

References Hartkamp, A. D., De Beurs, K., Stein, A., & White, J. W. (1999). Interpolation techniques for climate variables.

Moral, F. J. (2010). Comparison of different geostatistical approaches to map climate variables: application to precipitation. *International Journal of Climatology*, 30(4), 620-631

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