



Original software publication

DSCompare: Unleashing the potential of ocean and atmospheric data with a comparative analysis software

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ARTICLE INFO

Keywords:

Dataset validation
Dataset comparison
Analysis
Reanalysis
Observed data

ABSTRACT

Data validation is a crucial step in the analysis of any dataset, as it ensures its reliability and accuracy. In the field of scientific research, where data play a fundamental role in making informed decisions and drawing meaningful conclusions, the validation process becomes even more critical. In this context, the comparison of analysis and reanalysis data with observations serves as an effective method to assess the quality and consistency of datasets. This paper presents the DSCompare tool able to evaluate numerically simulated oceanographic and atmospheric datasets by comparing them with observed data through performing multiple statistical tests.

Code metadata

Current code version	V2.1
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2023-317
Permanent link to reproducible capsule	https://codeocean.com/capsule/9212622/tree/v1
Legal code license	MIT License
Code versioning system used	Zenodo
Software code languages, tools and services used	MATLAB
Compilation requirements, operating environments and dependencies	MATLAB 2021
If available, link to developer documentation/manual	https://zenodo.org/record/8152618/files/UserManual_DSCompare_v2.1.pdf?download=1
Support email for questions	humberto.varona@ufpe.br

1. Introduction

The oceans cover approximately 71% of the Earth's surface [1] and contain an incredible amount of information that scientists strive to unravel. However, obtaining comprehensive observational data from the vast oceanic poses numerous challenges. Consequently, researchers have turned to oceanic datasets analysis and reanalysis to gain insights into long-term trends, understand climate variability [2], and

predict future scenarios [3]. Nevertheless, these datasets must undergo rigorous validation to ensure their reliability and usability. Oceanic datasets analysis involves processing and interpreting a vast amount of collected data to derive meaningful insights into ocean dynamics and properties, such as temperature, salinity, currents, and biological activity. Reanalysis, on the other hand, refers to the reconstruction of past climate conditions using historical data and advanced mathematical models [4]. By assimilating various data sources, including in-situ

DOI of original article: <https://doi.org/10.1016/j.rsma.2023.103071>.

The code (and data) in this article has been certified as Reproducible by Code Ocean: (<https://codeocean.com/>). More information on the Reproducibility Badge Initiative is available at <https://www.elsevier.com/physical-sciences-and-engineering/computer-science/journals>.

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<https://doi.org/10.1016/j.simpa.2023.100578>

Received 29 June 2023; Received in revised form 28 August 2023; Accepted 3 September 2023

measurements, remote sensing, buoys, ships, and autonomous underwater vehicles, analysts and reanalysts create comprehensive datasets that provide valuable information about the state of the oceans. This software takes a comprehensive approach to validate ocean analysis and reanalysis datasets against observational data. Several statistical techniques commonly used by geoscientists, including bias analysis [5–8], root mean square error (RMSE) computations [5,8,9], scatter index [5,9,10], Mann Whitney test [11,12], two samples *t*-test [11,13], two samples *F*-test [14], trend [15], covariance, correlation and maximum anomaly analysis [16], are employed to assess the performance and consistency of the datasets. The evaluation focuses on comparing large-scale ocean patterns as well as localized regions and finer scales to detect possible discrepancies between datasets and observations.

2. Software details

The DSCompare software [17] has been developed in the App designer suit as a MATLAB 2021b package. Its main objective is to validate spatially distributed analysis and reanalysis datasets (model output) through comparisons with observed datasets using various statistical tests. This software only imports data that are in standard NetCDF format. As a first step the two datasets to be compared (simulated and observed) should be prepared, since both should have the same spatial resolution. This is done by interpolating the simulated dataset and obtaining a new grid with values at the same nodes as the observed dataset. Such step is automatically executed by DSCompare, after having uploaded both sets in the software. The simulated dataset must be vertically interpolated in order to match the observed data at the same depths. The latter can be achieved through the CDO (Climate Data Operator) [18] and NCVerticalInterp [19] tools. Also both datasets must have the same frequency and the same start and end dates, and by using CDO this process can be done very simply. For hydro-thermodynamics datasets an additional step is needed, since the output of models such as CROCO, ROMS, and NEMO are in specific NetCDF format, by adopting ad-hoc tools able to standardize them: CROCOTOOLS [20], ROMSTOOLS [21,22], and fcNEMOtoStd [23] respectively. In case the validation is performed on the ocean surface or at a specific depth, a specific plane (desired depth) can be selected with CDO and NCVerticalInterp. DSCompare is very easy to use, once compatibilized the two datasets to be compared (equal spatial resolution, where the grid nodes coincide, and equal frequency, coinciding the time instants, the initial and final dates). The simulated dataset (Dataset for Analysis) and the observed dataset (Reference Dataset) will be firstly loaded, then the next step will be to select the variables to compare (normally a NetCDF file has several variables, this process can be accelerated by previously extracting the variables in separate files with the CDO and NCO [24] tools). After this, DSCompare will automatically perform all the statistical analyses, which will be displayed by selecting the analysis using the button corresponding to it (Fig. 1).

3. Software algorithms

The DSCompare software automatically computes several statistical tests for both datasets (simulated and observed) after loading the NetCDF files and creating a time series at each node of both grids. The complete list of these statistical tests is as follows: Mean value of oceanographic parameters, Mann Whitney test, two-sample *t*-test, two-sample *F*-test, normalized bias/bias (Equations S1 and S2), standard deviation, coefficient of determination (Equation S3), RMSE (Equation S4), maximum anomalies, scatter index (Equation S5), covariance (Equation S6), and trend analysis. All these statistical tests are essential for analyzing, comparing, validating and interpreting data in ocean and atmospheric sciences. They provide researchers with valuable tools for exploring trends, comparing samples, analyzing distributions, and establishing relationships.

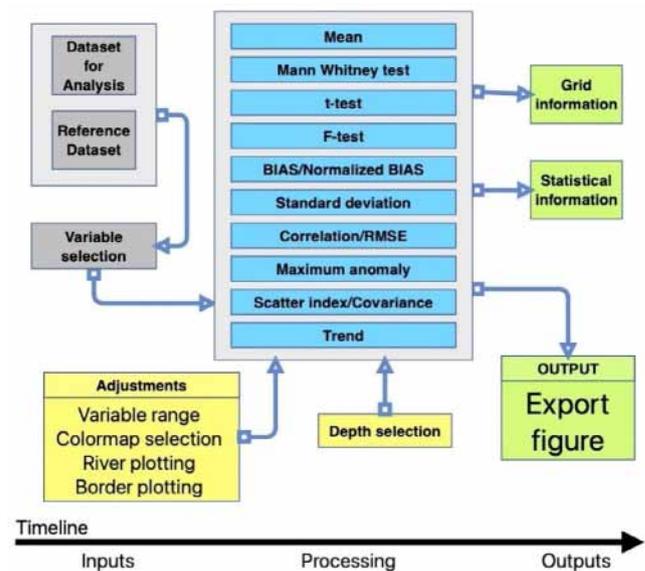


Fig. 1. Logical steps to perform ocean variable validation with DSCompare software.

4. Related works

Using DSCompare, spatial significant waveheight data, obtained in 3 study cases simulated with the WAVEWATCH III model during an extreme weather event occurred in March 2016 off the coast of Rio Grande do Sul (Brazil), have been validated, and the results of this research have been published [5].

5. Impact overview

The DSCompare software can be quickly and efficiently employed to validate numerically simulated datasets with different oceanic and atmospheric products. A large percentage of research in both oceanography and meteorology is performed on simulated datasets, which require validation before use. This is precisely where DSCompare plays an important role, saving time in validation and evaluating datasets from analysis and reanalysis. As a summary of the impact that this software can produce, let us explore these examples of its utilization.

Due to the fact that the GLOBAL_MULTIYEAR_PHY_001_030 product is a global reanalysis dataset [25] and has been used for the region of the waters adjacent to Fernando de Noronha Island (North-Eastern Brazil), it is validated at the surface and at various depths through vertical profiles by computing the bias (mean value of the difference between the observed data and the reanalysis data [26]). The surface validations have been performed with the DSCompare v2.0 software, using the MODIS Aqua satellite Sea Surface Temperature (SST) datasets [27,28], Sea Surface Salinity (SSS) from the SMOS mission dataset (Soil Moisture and Ocean Salinity [29]) and surface current data from the OSCAR dataset (Ocean Surface Currents Analyses Real-time; [30]). The latter product was used by [31] within a study of surface currents in the tropical Atlantic Ocean; OSCAR is a reliable data set, which computes surface current velocity from satellite data combined with in-situ instrument data of Sea Surface Height (SSH), SST and surface winds. The parameters SSS, SST, and surface current components of the GLOBAL_MULTIYEAR_PHY_001_030 product were validated by computing the BIAS with respect to the SMOS, MODIS-Aqua, and OSCAR datasets (Figure S1), showing good agreement at the **surface** for this region. The maximum bias for the SSS, SST, and the zonal and meridional components of the surface currents were 0.15 psu, 0.2 °C, 0.11 m s⁻¹, and 0.15 m s⁻¹ respectively.

Figure S2 shows the spatial comparison between the GFS model output [32] in the area located within 70°W – 4°W of longitude and

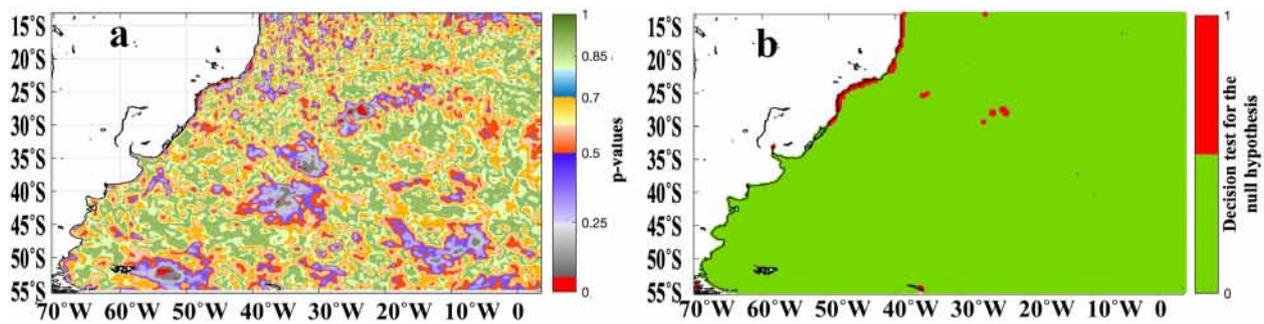


Fig. 2. Comparison between the GFS wind model and the ASCAT dataset: (a) is the probability (p -values) resulting from the t -test with a significance value of 0.05, and (b) is the result of the t -test hypothesis evaluation (0 is accepted and 1 is rejected).

55°S - 13°S of latitude and the ASCAT satellite retrieved dataset [33], this type of study was performed at [5] to validate the wind data from the GFS model before being used as input to the WAVWATCHIII model. The GFS data, in general compare well with the ASCAT dataset (Table S1): the mean values of bias and RMSE are shown in the whole region for the wind components and their intensity, and can be also seen in Figure S2a-f. On the contrary, along a stretch of the Rio Grande do Sul coast there is an overestimation of the wind intensity, as shown in Fig. 2a, b where significant differences between the GFS and ASCAT models can be acknowledged. This can be explained by the fact that the remotely sensed wind datasets are altimetric and these are affected by 25%–30% of error within the coastal areas due to different sources.

Among the most common sources of error are the following: Atmospheric effects, such as atmospheric pressure and water vapor, can cause significant errors in satellite altimetry. Changes in atmospheric pressure can affect the measurement of sea level, while water vapor can cause errors in the microwave signals used to measure the waves [34]. Studies have shown that atmospheric effects can cause errors of up to 10% in wave height measurements; Wind can also affect the accuracy of wave measurements obtained through satellite altimetry. Strong winds can cause significant waveheight and wavelength changes, making it difficult to obtain accurate measurements. Moreover, the wind can cause the ocean's surface to become rough [34,35], leading to errors in the satellite measurements and accounting for up to 15% in waveheight measurements' error; Satellite orbit errors can also affect the accuracy of wave measurements obtained through satellite altimetry. These errors can be caused by various factors, such as gravitational forces and drag forces from the atmosphere. Studies have shown that orbit errors can cause errors of up to 3 cm in sea level measurements [36,37]; and Instrumental errors can also affect the accuracy of wave measurements obtained through satellite altimetry and can be due to various factors, such as calibration errors and electronic noise [35,37]. Instrumental errors can cause errors of up to 1 cm in sea level measurements.

Fig. 3 shows the comparison of SST between the ERA5 and Windsat datasets. The entire region shows that there are no significant differences according to the Mann-Whitney test all p -values > 0.05 (Fig. 3a), however Fig. 3b shows large absolute bias values on the west coast of Africa, in the vicinity of the 3°S parallel, and in areas near the east coast of South America between the 50°S to 20°S parallels. Fig. 3c shows the spatial distribution of the maximum SST anomalies, calculated according to the method of [38], finding anomalies of 4 to 5 °C between the 50°S and 25°S parallels, and north of 28°N.

mStatGraph has 10 data comparison tests that in together with the loading of each dataset to be compared have a run time of $O(n^2)$ each. Table S2 shows the performance of mStatGraph in terms of processing time and RAM usage in the 6 examples provided. The code is optimized to minimize RAM usage so that only the two variables to be compared are loaded, regardless of how many variables are contained in the NetCDF files of the datasets to be analyzed and the reference one.

6. Further development of the software

In the next future, the following equations will be implemented to have more comparison criteria between simulated and observed spatial datasets: The Mean Bias Error [39], is computed by Equation S7; The normalized Root Mean Square Error [40], this parameter can be computed by the equations S8 and S9.; the Percentage Error (Equation S10) [40]; and the Model Performance Index (Equation S11) [41].

7. Final remarks

This software can be widely used in a practical and efficient manner for various types of ocean or atmospheric research application where it is necessary to validate simulated datasets from analysis and reanalysis by comparing them with observed data.

CRediT authorship contribution statement

H.L. Varona: Conceptualization, Methodology, Software, Validation, Formal analysis, Visualization, Writing – original draft, Writing – review & editing. **T.A. Capuano:** Software, Visualization, Writing – original draft. **C. Noriega:** Visualization, Writing – original draft, Writing – review & editing. **J. Araujo:** Visualization, Writing – original draft, Writing – review & editing. **M. Araujo:** Conceptualization, Methodology, Writing – review & editing, Supervision, Funding acquisition. **F. Hernandez:** Methodology, Visualization, Software.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

HLV acknowledges the TRIATLAS project, which has received funding from the European Union's Horizon 2020 Research and Innovation Program under grant agreement no. 817578. CN acknowledges the Fade/UFPE, Brazil agreement no. 04/2018 (5850.0108524.18.9) through grant postdoctoral stage (UFPE), Brazil. JA and MA acknowledge the support of the Brazilian Research Network on Global Climate Change-Rede CLIMA, Brazil (FINEP grants 01.13.0353-00), and to the International Joint Laboratory TAPIOCA (IRD-UFPE-UFRPE), Brazil.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.simpa.2023.100578>.

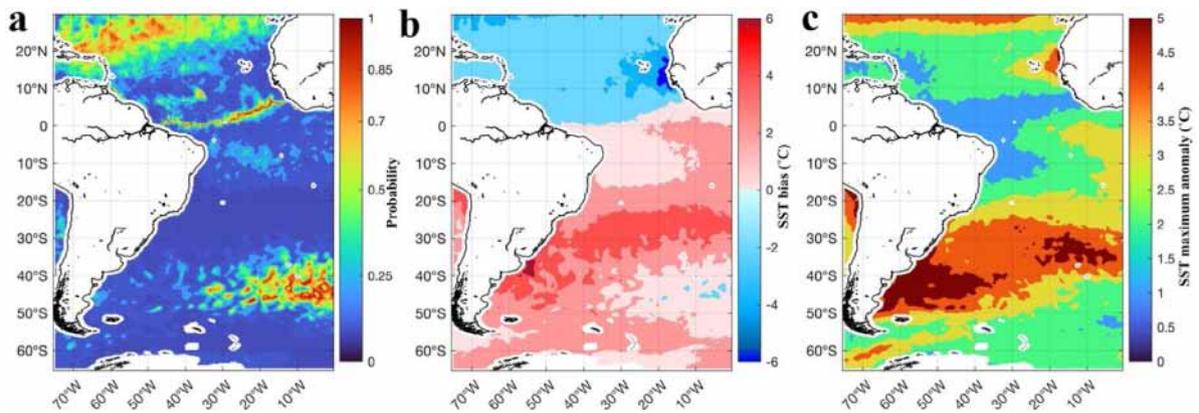


Fig. 3. Comparison between ERA5 SST and Windsat SST: (a) Probability of Mann-Whitney test, (b) SST bias and (c) SST maximum anomaly.

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