eva3dm: A R-package for model evaluation of 3D weather and air quality models

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Summary

Eva3dm is a package designed to support the evaluation of 3-dimensional physical models (particularly, weather and air quality models) against observation data in order to quantify different errors and bias present in the model results.

Statement of need

Evaluation is a crucial step in any model application, as it ensures that the model results accurately represent the variables of interest. Without a good evaluation process, the reliability and applicability of model outputs remain uncertain. There are currently other tools available in R (Carslaw & Ropkins, 2012), Python (Ladwig, 2017) and other languages (Appel, 2011; NCAR et al., 2017). However, these tools often focus on specific aspects (data visualization, geoprocessing, etc) and lack a fully integrated framework. This package fills that gap by streamlining the entire evaluation process—from preprocessing observations and model outputs to statistical analysis and visualization—offering a comprehensive and user-friendly solution for air quality model assessment.

Description

The literature presents various evaluation criteria depending on the evaluated variable (C. A. Emery & Tai, 2001; C. et. al Emery, 2017; Monk, 2019; Zhai, 2024; Zhang, 2019), which can be used to compare models and assess their performance. These criteria vary based on the simulation goal, observation variability, and measurement errors.

A brief description of the steps to perform a model evaluation and the functions to support these steps are described in the next sections and Figure 1 shows a diagram of the workflow.
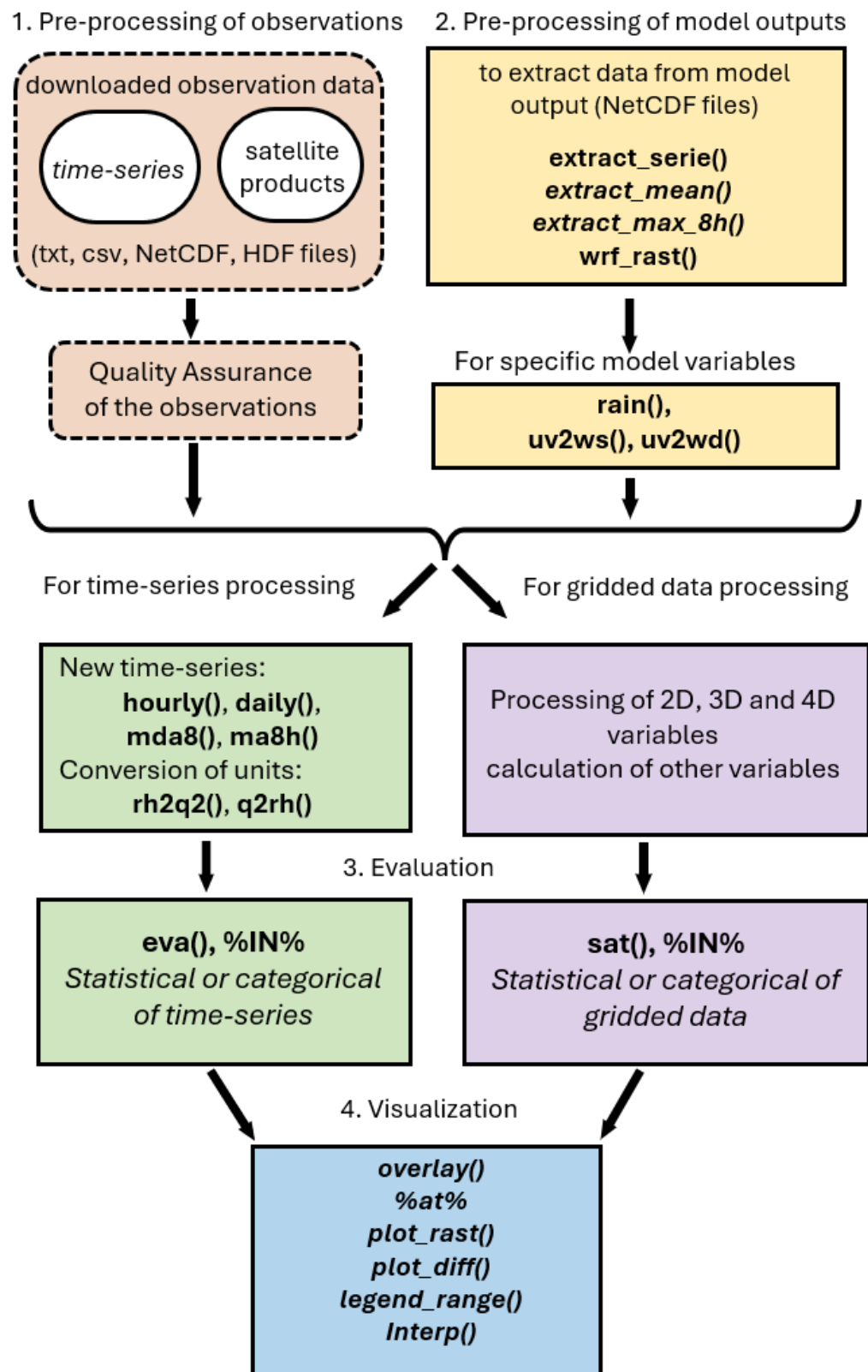
Figure 1: Diagram of the evaluation processs.

1. **Pre-processing of observations**

- Download the observations, some examples include:

    - METAR (METeorological Aerodrome Report) can be downloaded using the R-package riem or the Iowa State University website
    - AERONET (Aerosol Robotic Network) can be downloaded at AErosol RObotic NETwork website
    - Air Quality data for Brazil can be downloaded using the R-package qualR, or QUALAR and MonitorAir websites
    - Satellite products are available at the NASA Giovanni website

- Process observation data for evaluation: Unit conversion, time zone conversion to UTC, and calculation of secondary variables. The functions rh2q and q2rh convert humidity units and the functions mda8, ma8h, hourly, and daily can be used to calculate average of time-series. The format used to evaluate time-series is a data.frame, the first column must contain time (in POSIXlt) and one additional column for each different location, satellite data can be read using the function rast from R-package terra.

- Quality Assurance of the observation data: check for values outside the valid range, check if the data is available for the time-period and region of the simulation and note any singular event.

2. **Pre-processing of model outputs**

Extraction of model outputs, unit conversion and calculation of secondary variables.

The function extract_serie extract and save time-series from model outputs using a data.frame with name of the location (row names), latitude (column lat) and longitude (column lon), while the functions extract_mean and extract_max_8h extract the average or the daily maximum of 8-hour moving average and save in a new NetCDF file.

The function wrf_rast can be used to read model output and return a SpatRaster or SpatVector object from the model files and its counterpart rast_to_netcdf that converts a SpatRaster to an array and/or save to an existing NetCDF file.

The functions uv2ws and uv2wd can be used to calculate wind speed and velocity from the model wind components (eastward and northward components) and the function rain can be used to calculate hourly precipitation from model accumulated precipitation variables.

3. **Model evaluation functions:**

The evaluation involves pairing observations with model results and calculating the statistical and/or categorical indexes.

There are two high level evaluation functions implemented in the package: eva and sat. The eva function performs the temporal pairing of both model and observation time-series by station (or combines all data). The sat function interpolates and pairs data in regular grids. Both functions call the low-level evaluation functions: stat to compute statistical metrics and cate to calculate categorical metrics based on a threshold value. These result can be written and read using the write_stat and read_stat functions.

4. **Visualization and extractting information functions**

Visualization of model results and statistical results.

There are functions for visualization, interpolation and to extract information from NetCDF files, Table 1 list these functions.

Schuch. (2025). eva3dm: A R-package for model evaluation of 3D weather and air quality models. *Journal of Open Source Software*, *10*(108), 7797. https://doi.org/10.21105/joss.07797.

Table 1: Visualization, interpolation and information functions.

Function name	Description
plot_rast	Custom plot for SpatRaster objects
plot_diff	Custom plot for absolute or relative difference of two SpatRaster objects
overlay	Custom plot to overlay points
legend_range	Custom legend that displays max, min and average
interp	Interpolation function that combines project and resample for SpatRaster objects
ncdump	Print a ncdump -h equivalent command for a NetCDF file
vars	Return the name of the variables on NetCDF file
atr	Read and write attributes from a Netcdf file

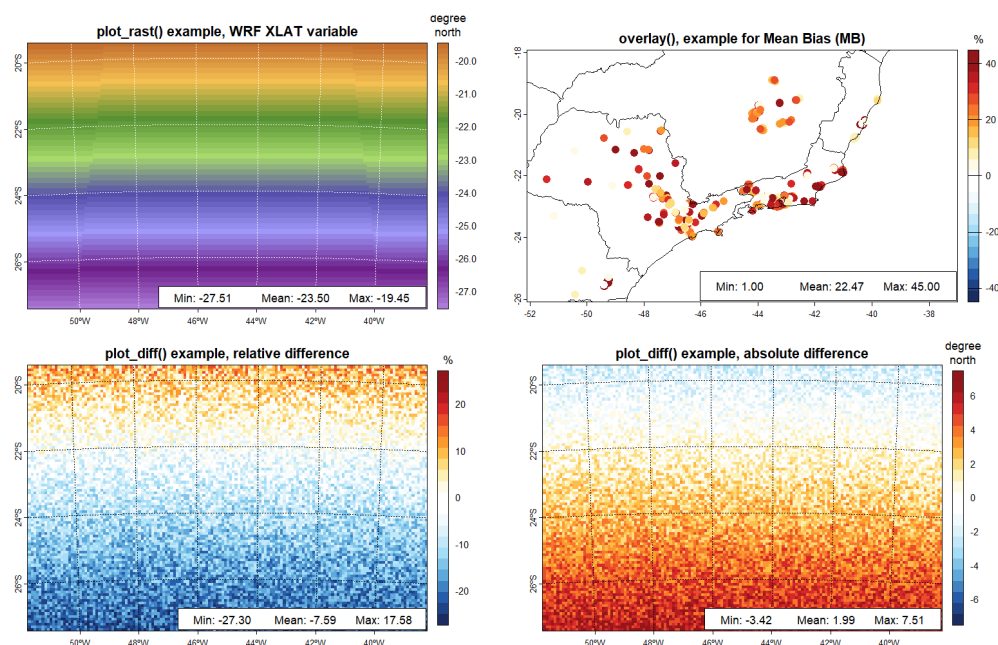Figure 2 shows examples of the first 4 functions on Table 1:

Figure 2: Example from the viasualization functions.

Bellow is presented a simple example of evaluation of temperature from WRF-Chem using METAR data.

```
library(eva3dm)

# folder with the data for this example
f          <- system.file("extdata",package="eva3dm")
# opening an example of observation from METAR, in degree Celsius
OBS        <- readRDS(paste0(f,"/metar.T2.Rds"))
# openeing data extracted from WRF-Chem model using extract_serie()
MODEL      <- readRDS(paste0(f,"/model.d03.T2.Rds"))
# converting from Kelving to Celcius
MODEL[-1] <- MODEL[-1] - 273.15
# perform the model evaluation
```

```
evaluation <- eva(mo = MODEL, ob = OBS, rname = 'T2 from WRF-Chem')
print(evaluation)
```

Special functions:

Table 2: Special functions.

Function name	Description	Objective
`%at%`	Combine a data.frame containing evaluation results and a data.frame containing geographical coordinates (site list)	To georeference the statistical results for visualization
`%IN%`	Filter a observation data.frame based on model time-series data.frame. Also can be used to crop a `SpatRaster` based on a second `SpatRaster`	To compare results from simulation with different domains
`template`	Create folders, post-processing and evaluation scripts	Templates to process and evaluate multiple variables from one or multiple simulations

Note that the examples from eva3dm are focused on the Weather Research and Forecasting coupled with Chemistry WRF-Chem (Grell, 2005), but the package can be applied to other models, such as CMAQ, CAMx, WACCM and CAM-Chem. More details can be found in the package documentation and vignettes.

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