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pyDARTdiags: A Python package for manipulating observation sequences and calculating observation-space diagnostics for the Data Assimilation Research Testbed (DART)

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Summary

pyDARTdiags is a Python package for manipulating observation sequences and calculating observation-space diagnostics for the Data Assimilation Research Testbed (DART) (J. Anderson et al., 2009; Gharamti et al., 2025; UCAR/NSF NCAR/CISL/DAReS, 2025).

Data assimilation is a scientific technique that combines observations (such as measurements from weather satellites, buoys, radar, or other sensors) with predictions from numerical models to produce an improved estimate of the state of a system (J. L. Anderson, 2009; Evensen, 2003). It is widely used in fields like meteorology, oceanography, hydrology, and environmental science.

During assimilation, the model state is transformed into observation space by interpolating the model state to each observation location. Observation space diagnostics are used to visualize observations and model predictions (in observation space), and compare their statistical properties both before and after assimilation. Thereby, these diagnostics are key tools to model evaluation and prediction tasks.

The Data Assimilation Research Testbed (DART) is a widely used community software facility for ensemble data assimilation. pyDARTdiags is a Python package for manipulating observation sequences and calculating observation-space diagnostics for DART. It provides tools to read, manipulate,and analyze DART observation sequence files using familiar, modern Python libraries. With pyDARTdiags, users can extract data, compute diagnostics, and create visualizations, all within reproducible Python workflows that integrate seamlessly with the broader scientific ecosystem.

Statement of need

DART merges diverse and complex observations into an internal data format called “observation sequence” files, which inherit metadata from each observation. Observation sequence files including the model states are also generated, wherein the model states have been transformed into the observation space for direct comparisons and analysis. While DART provides robust tools for data assimilation, its observation sequence files are not easily accessible for users wishing to perform custom diagnostics or integrate with Python-based workflows.

DART’s observation sequence files are central to its workflow, but their format and complexity can make them challenging to manipulate and analyze outside of the DART ecosystem. Existing DART tools for calculation of observation-space diagnostics are written in Fortran with visualization in MATLAB, which may not be freely accessible to all users. To manipulate and analyze the data using open-source tools a converter/interface is required. pyDARTdiags is a Python package created to address this need by providing a single package to process and visualize observation space diagnostics.

PyDARTdiags ingests observation sequences into an ObsSequence object which contains the metadata about an observation sequence and a pandas DataFrame (The pandas development team, 2025) containing all the data for the observations.

This provides several advantages over the existing Fortran+MATLAB DART software:

- Providing Python routines for reading and writing DART observation sequence files allows for the manipulation of observation sequences interactively via DataFrames using popular, open-source data science libraries.
- Synthesizing the manipulation, analysis, and visualization of observation sequence files into a single Python workflow improves portability and flexibility over the fractured Fortran/MATLAB workflow.
- Enabling calculation of observation-space statistics (e.g., RMSE, bias, total spread) on a DataFrame enables Data Assimilation researchers and users to write custom diagnostics based on DataFrames. By decoupling the observation sequence file format from the DataFrame-based analysis, pyDARTdiags ensures that updates to the DART file format do not disrupt user-created diagnostic routines.
- Supporting both static (via Matplotlib, Hunter, 2007; McKinney, 2010) and interactive (via Plotly, Plotly Technologies Inc., 2015) plotting, facilitates the processing of observational datasets, quality control, and gaining insights about the spatial distribution of outliers or other (technical) anomalies.
- Facilitating reproducible, scriptable workflows for observation-space diagnostics enables the inclusion in Jupyter notebook workflows. A concrete use case is its integration into the the CESM Regional Ocean and Carbon Configurator with Data Assimilation and Embedding (CROCODILE, CROCODILE-CESM, 2025) project, which is a community platform for accelerating observationally-constrained regional ocean modeling. pyDARTdiags is used for observation space diagnostics and model-to-observation comparison in the Jupyter notebook workflows for this project.

Examples for manipulating observation sequences, visualizing observational data, and generating diagnostic plots can be found in the pyDARTdiags examples gallery. A detailed description of the available diagnostic statistics and available plotting functions is provided in the user guide. The pyDARTdiags source code is available at https://github.com/NCAR/pyDARTdiags.

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