EGU26-1991, updated on 20 May 2026
https://doi.org/10.5194/egusphere-egu26-1991
EGU General Assembly 2026

Reconstructing GRACE Terrestrial Water Storage Anomalies time series using Bias-Aware Machine Learning

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A commonly known limitation in the use of GRACE data is the one-year (July 2017 to May 2018) gap between the end of the GRACE mission and the beginning of the GRACE-FO operation. In this study, we reconstructed total water storage (TWS) at the grid-cell scale using two modeling approaches: a Bias-Aware Machine Learning (ML) model and an autoregressive integrated moving average (ARIMA) model with exogenous variables. Both approaches were applied to CSR mascon GRACE data to reconstruct missing monthly observations. Bias-Aware ML represents a new paradigm of optimal algorithm design, model architecture, and aimed at explicitly detecting, measuring, and mitigating bias in data, models, or outputs.

We applied this approach to the transboundary Bug River Basin (BRB), which spans Poland, Ukraine, and Belarus. An XGBoost ML model was used with multiple groups of high-resolution (0.1°) hydrometeorological variables—precipitation, soil moisture, evapotranspiration, river runoff, and land surface temperature—together with static physiographic variables (elevation, lithology, and land cover) as predictors.

The XGBoost model explains approximately 86% of the variance in GRACE TWS values on unseen test data. Model performance relies strongly on short-term memory, with the TWS rolling average being the most influential predictor. Seasonal variability is well captured; however, the model tends to overestimate TWS in the northern and northwestern regions and underestimate it in the eastern and southeastern areas. Overall performance shows a slight west-to-east decline. Model performance deteriorates for extreme TWS values, indicating limited skill in representing hydrological extremes.

The results indicate that gap filling supported by bias-aware ML substantially outperformed seasonal ARIMA with exogenous variables across the BRB. The correlation coefficient with *in situ* observations increased from 0.30 to 0.74. We showed that the use of bias-aware ML with engineered predictos, combined with a post-processing stacking framework, provides a significant advantage over traditional extrapolation-based algorithms. We further showed that the trained ML models learned complex relationships between the input datasets and GRACE-derived TWS, resulting in improved performance of the reconstructed GRACE time series. The results of this

study are expected to serve as a benchmark for filling data gaps between the GRACE and GRACE-FO missions and for selecting appropriate GRACE solutions for regional hydrological studies.

The study was conducted as part of the project GRANDE-U “Groundwater Resilience Assessment through iNtegrated Data Exploration for Ukraine” (NSF Awards No. 2409395 and 2409396). Vilnius University has received funding from the Research Council of Lithuania (LMTLT), agreement No. S-IMPRESSU-24-3.