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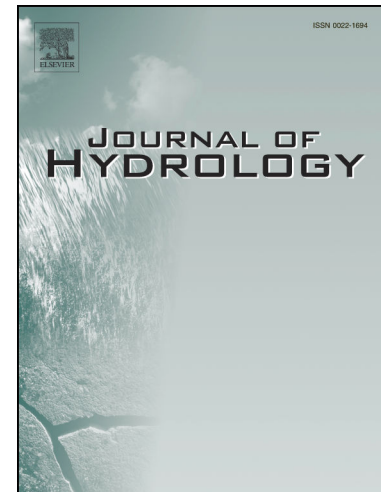
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1 Machine learning assessment of hydrological model performance under localized water 2 storage changes through downscaling

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11

12 Abstract

13 The coarse spatial resolution of the Gravity Recovery and Climate Experiment (GRACE) data
14 has limited its application in the management of local-scale water resources. To address this
15 limitation, we developed a new downscaling approach using predictors from regional and
16 global hydrological models for a 15-year period (2002-2017) and tested it in the northern Great
17 Artesian Basin, Australia. We used four different machine learning algorithms (support vector
18 machine, partial least squares, gaussian process and random forest) to downscale the original
19 GRACE estimate of 0.5° to a spatial grain size of 0.1° (global) and 0.05° (regional). This was
20 based on precipitation, evapotranspiration and runoff estimates from the Famine Early Warning
21 Systems Network Land Data Assimilation System (FLDAS) and Australian Water Outlook
22 (AWO) hydrological models, respectively. The downscaled products were validated using 42
23 in-situ precipitation observations spread across the test region. We further evaluated which of
24 the downscaled products best mimicked local-scale hydrology using a range of statistical
25 metrics. Our results showed that regional hydrological models best characterized the dynamics
26 of local scale hydrology (rainfall v. downscaled product), and the gaussian process regression
27 algorithm made the best predictions for both models. The correlation coefficients for the raw
28 values varied from 0.45 to 0.49 while that of the standardized values varied from 0.46 to 0.52
29 with the random forest model providing the best fitting for the regional-based products. The
30 regional downscaling approach employed in this study may be readily integrated into local
31 water resources planning programs.

32 1. Introduction

33 The emerging assessment of catchment-scale water resources under a changing climate has
34 intensified the need to bridge the spatial scale gap between coarse GRACE- Terrestrial Water
35 Storage (TWS) estimates and local scale hydro-climatic variables through downscaling
36 (Atkinson, 2013; Sachindra et al., 2018). Presently, the two major methods for downscaling are
37 dynamic and statistical downscaling (Yin et al., 2018). While dynamic downscaling techniques
38 are used in building regional numerical models at finer spatial resolutions, statistical
39 downscaling applies historical observations to derive relationships between large-scale climate
40 factors and local-scale hydrological variables (Ndehedehe, 2022a). This provides the capacity
41 to flexibly build models and incorporate high-resolution modelling factors to improve the
42 spatial resolution of the response variable. These high-resolution modelling factors can be

43 acquired from either regional or global hydrological models. The entire statistical downscaling
44 process is aimed at providing finer details of a hydrological estimate (in our case, GRACE-
45 TWS), which best depicts the local scale hydrology of the region of interest. It is thus pertinent
46 to compare the outputs from regional and global hydrological models to improve understanding
47 of which provides the best estimate for local-scale terrestrial water storage assessments. [Wilby
48 et al. \(2004\)](#) sub-divided statistical downscaling approaches into three categories: weather
49 classification-based approaches, weather generators and regression-based approaches. Of the
50 three, the latter has gained the most popularity and application due to its simplicity. The
51 regression techniques widely used in statistical downscaling include multi-linear regression,
52 generalized linear models, artificial neural networks, support vector machines, partial least
53 squares regression etc ([Sachindra et al., 2014](#); [Beecham et al., 2014](#); [Ahmed et al., 2015](#); [Goly
54 et al., 2014](#); [Vishwakarma et al., 2021](#)). Due to their learning and prediction capabilities, they
55 are often referred to as machine learning methods.

56 Machine learning methods like regression and neural networks can effectively solve non-linear
57 problems and simulate complex hydrological processes. This makes them well-suited for
58 downscaling applications ([Tao et al., 2023](#)). For example, [Vishwakarma et al., \(2021\)](#) exploited
59 dominant common statistical modes between high resolution datasets from global hydrological
60 models to improve the spatial resolution of global GRACE-TWS using partial least squares
61 regression. The efficacy of their downscaled products for the 160 catchments explored in their
62 study was evaluated by using their individual conservation of mass. Using an empirical
63 regression model, [Ning et al. \(2014\)](#) developed an integrated downscaled product of GRACE-
64 TWS at 0.25° scale from global hydrological models. The downscaled product was validated
65 against in-situ groundwater levels over the Yunnan province, China. Apart from global
66 hydrological models, the work undertaken by [Miro and Famiglietti \(2018\)](#) revealed the
67 potential of regional hydrological models in machine learning (artificial neural network)
68 downscaling of GRACE products. Using high resolution groundwater storage changes from
69 the San Joaquin valley in California, their work demonstrated the flexibility of the method and
70 datasets in accurately reproducing local groundwater trends and its heterogenous behaviour.
71 Furthermore, [He et al. \(2021\)](#) developed three convoluted neural network (CNN) - based
72 frameworks to downscale the GRACE-TWS from 110km to 10km using simulations from the
73 Ecological Assimilation of Land and Climate Observation (EALCO) regional hydrological
74 model and compared the outputs of the CNN-based methods with the empirical linear
75 regression-based downscaling method. These studies explored the use of high-resolution global
76 and regional hydrological models in their downscaling approach. They also demonstrate the
77 benefits (e.g., simplicity, flexibility etc.) associated with each machine learning technique in
78 advancing knowledge on the downscaling of GRACE products. However, there is still
79 uncertainty as to how downscaled products mimic local scale hydrological fluxes and patterns
80 (catchment-based land water storage changes) to enable us determine which hydrological
81 model and machine learning method best suits the downscaling operation. Very few studies
82 have employed a hybrid approach that combines the strengths of both global and regional
83 hydrological models in downscaling (e.g., [Seyoum et al., 2019](#)). Such an integrated approach
84 can potentially provide more robust and accurate downscaling results, especially when dealing
85 with regions that are subject to diverse hydrological conditions and require a comprehensive
86 understanding of both large-scale and small-scale dynamics. However, for the purpose of this
87 study, we limit our experiments to global and regional hydrological models.

88 Global hydrological models (GHMs) have emerged as a critical tool in analysing complex,
89 large-scale hydrological systems and predicting the distribution, availability, and movement of
90 water resources globally. Their broad coverage provides them with a consistent framework for

91 hydrological simulations across different regions and enables them to capture large-scale
92 climate patterns and trends. This has made them very popular in statistical downscaling
93 operations of GRACE- Δ TWS estimates (e.g., Vishwakarma et al., 2021; Ning et al., 2014; Yin
94 et al., 2018). Regional hydrological models (RHMs) on the other hand provide detailed, high-
95 resolution simulations at a regional or local scale. They capture fine-scale hydrological
96 processes, topography, land use and other factors that influence water availability and
97 movement. Their incorporation of local data and observations makes it easier to represent the
98 unique characteristics of specific regions leading to a more realistic representation of regional
99 hydrological processes. Global and regional hydrological models share some similar
100 characteristics but also have distinguishing features. These features can include varying
101 hydrological scales, focus areas, specific purposes and land surface modelling modes (i.e.,
102 climate inputs and post processing techniques). In this study, our emphasis is to examine the
103 effects of these characteristics in land water storage assessments by downscaling with high
104 resolution predictors from both model types. Regional hydrological downscaling produces
105 higher spatial resolution and provides detailed designs aimed at capturing local hydrological
106 processes. However, their downscaling is strongly dependent on the lateral boundary
107 conditions and the techniques used to constrain the high-resolution predictors to the coarse
108 scale predictand. The large-scale errors inherent in the coarse scale predictands tends to be
109 retained in the downscaled model, thus increasing the risk of overfitting and uncertainty
110 amplification (Pielke & Wilby, 2012). On the other hand, global hydrological models which
111 best characterizes large-geographical extents maintains a consistent modelling approach with
112 GRACE-TWS and ensures uniformity in the analysis of TWS variations leading to a better
113 quantification and propagation of uncertainties in the model output (Güntner, 2008). To have a
114 better understanding of our downscaling process and final products, we applied four well-
115 known regression models on both the global and regional downscaling models. To estimate the
116 performance of our downscaled products over local-scale hydrology, we compared the
117 downscaled estimate from each method and model to in-situ precipitation estimates over the
118 study region and period. The importance of precipitation in validation was warranted as several
119 studies have reported its role as the most dominant forcing mechanism responsible for the
120 spatio-temporal variations of GRACE TWS in tropical and temperate regions (e.g., Song et al.,
121 2015; Rodell et al., 2018 Meng et al., 2019; Yin et al., 2020; Kalu et al., 2021, 2022).

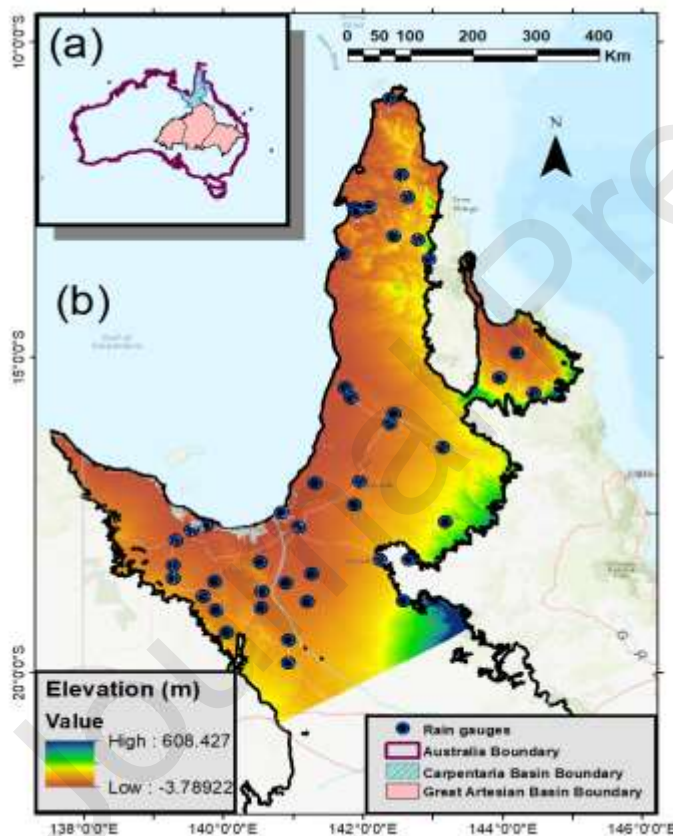
122 The key objective is to evaluate which hydrological model and machine learning method
123 provides the most accurate downscaled water storage estimates compared to local-scale
124 hydrological flux changes. To achieve this, we employed high spatial-resolution datasets from
125 both global and regional hydrological models to perform a statistical downscaling of GRACE-
126 TWS using various regression-based approaches. The downscaled products from both models
127 were evaluated against in-situ based precipitation patterns over the study region to provide
128 insights as to which model best characterizes local-scale hydrology. By local-scale hydrology,
129 we mean the dynamics of land water storage changes induced by hydrological flux variables
130 over a small catchment. We also make suggestions on the preferred model and method for
131 regional Δ TWS downscaling operations.

132 2. Study region and data

133 The Carpentaria Basin (CB) is located in northern Australia and situated at the northern part of
134 the Great Artesian Basin (Fig. 1) with an estimated area of 300,000 km². Its climate is
135 influenced by monsoonal patterns of tropical northern Australia resulting in distinct wet and
136 dry seasons. Our choice of the CB as a suitable test region was to provide a more
137 comprehensive understanding of freshwater dynamics, its availability, and the impacts of

138 climate variability across a wet-dry climate zone. This knowledge is vital for sustainable water
 139 management, ecosystem preservation, and mitigating water-related challenges in diverse
 140 environments.

141 The climatic condition of the Carpentaria Basin is hot and humid with two seasons per year.
 142 The dry season runs from May to October and is characterized by lower rainfall and higher
 143 temperatures. During this period, water sources may become more limited, and some areas may
 144 experience reduced water availability, fire risks, and drought conditions (Kaushik et al., 2021).
 145 On the other hand, the wet season occurs from November to April. During this time, the region
 146 receives heavy rainfall due to the monsoon winds and the convergence of moist air masses.
 147 These rains are crucial for replenishing water bodies, supporting vegetation growth and
 148 maintaining ecological balance. Almost all the rains are compressed into two or three months,
 149 and during this period many low-lying areas are flooded. A large portion of the CB comprises
 150 floodplains, with very low relief (Fig. 1), resulting in significant tidal inundation during the
 151 wet season. More than 80% of the annual rainfall results in large, inundated areas of these
 152 floodplains, much of which recede relatively rapidly, in some downstream areas (Ndehedehe
 153 et al., 2021)



154

155 Fig 1. Study area map showing (a) the situation of the CB in Australia and (b) the topography
 156 of the test region in the northern Great Artesian Basin, Australia and the location of the rain
 157 gauges used for validation and local-scale assessment. (The ground surface topography data
 158 used for this figure was gotten from the Australian Smoothed Digital Elevation Model which
 159 has been smoothed to reduce noise and improve the representation of surface shape).

160 In recent years, the CB, like many other regions around the world has been affected by the
 161 impacts of climate change (CSIRO, 2019). Changes in precipitation patterns, increased

162 temperatures, and more intense weather events can influence the basin's hydrology, affecting
163 water availability and the productivity of freshwater habitats by limiting flows, which supply
164 nutrients and supports the movement of fisheries from floodplain environments to marine
165 systems (Ndehedehe et al., 2021). Using the CB as a study region, our analysis provides more
166 insight into the climate and hydrology of the region to ensure sustainability of water resources,
167 protect ecosystem services and support the livelihood of local communities.

168 2.1 GRACE data

169 For this study, we used GRACE level 3 mascon products from the centre for space research
170 (CSR) of the University of Texas, Austin (Save et al., 2016) to quantify changes in terrestrial
171 water storage. The GRACE level 3 mascon products used in this study covered a total period
172 of 183 months, spanning from April 2002 to June 2017. Data gaps for months within our study
173 period were resolved using cubic interpolation for cases where more than two consecutive
174 solutions were missing. For single missing months (for e.g., June 2003, Jan 2011, May 2012,
175 Oct 2012), their values were interpolated by averaging the values of 2 months before and after
176 the month with missing data (e.g., Long et al., 2015; Yin et al., 2018). It is important to note
177 that GRACE dataset at 1.0 °, 0.5 ° and even 0.25° represent spatially interpolated quantities of
178 a coarser GRACE sample. This means that these available high resolution GRACE products
179 do not contain any new physical information at a spatial scale better than the native resolution
180 (see Luthcke et al., 2013; Watkins et al., 2015; Vishwakarma et al., 2021). Therefore, the choice
181 of which GRACE sample was used for the experiment may not directly affect the results of our
182 regression-based downscaling operation which aims at the introduction of new hydrological
183 variables to GRACE-TWS at higher resolutions. For our study, we used the filtered and
184 processed samples of the nominal GRACE dataset, which was provided at a $0.5^\circ \times 0.5^\circ$ grid
185 cell for our experiment.

186 2.2 Global model (FLDAS data)

187 The Famine Early Warning Systems Network Land Data Assimilation System (FLDAS) is a
188 collaborative data assimilation project involving the U.S. Geological Survey (USGS), the
189 University of California Santa Barbara (UCSB) Climate Hazards Group (CHG), NASA
190 Goddard Space Flight Centre (GSFC) and the Earth Resources Observation and Science
191 (EROS) centre (Khorrani et al., 2023). By integrating remotely sensed, modelled, and in-situ
192 observations, FLDAS simulates different hydrological variables at a global scale. Our
193 hydrological variables of interest were precipitation, evapotranspiration and runoff datasets
194 from the Noah 3.6.1 model simulations with a spatial resolution of 0.10 degrees. The
195 simulations were forced by a combination of the Modern-Era Retrospective analysis for
196 Research and Applications version 2 (MERRA-2) data and Climate Hazards Group InfraRed
197 Precipitation with Station (CHIRPS) 6-hourly rainfall data to produce high resolution datasets.
198 These high-resolution predictors were extracted from the FLDAS-Noah and integrated into our
199 downscaling algorithms to produce finer-scale resolutions of Δ TWS over our test region.

200 2.3 Regional model (AWO data)

201 The Australian Water Outlook (AWO) is a regional water balance model based on the landscape
202 component of the Australian Water Resource Assessment system (AWRA-L). The model is a
203 one-dimensional grid-based water balance model that has a semi-distributed representation of
204 the soil, groundwater, and surface water stores. The AWO system incorporates a wide range of
205 climate inputs, downscaling techniques, post processing and assimilation of near real time
206 satellite soil moisture states as inputs to the AWRA-L model (Van Dijk, 2010; Frost & Shokri,

207 2021), to provide a consistent set of hydrological outputs at 0.05° grids across Australia. Our
 208 high-resolution predictor datasets of interest were precipitation, evapotranspiration, and runoff
 209 datasets. These were used to perform a statistical downscaling of Δ TWS over our test region,
 210 which was validated using in-situ precipitation data (section 2.4).

211 2.4 In-situ data

212 In this study, monthly precipitation values of 42-gauge stations in the CB from April 2002 to
 213 June 2017 were collected from the Australian Bureau of Meteorology (BOM). This data
 214 represents the local scale hydro-climatology of our test region. The rain gauges are almost
 215 uniformly distributed over our test region, though with a concentration to the lower part of our
 216 study area, and their locations are shown in Fig 1. The rain gauge time series generated from
 217 this dataset is the arithmetic average of all the gauges within our test region used in our
 218 experiment. Overall, the in-situ datasets for the 42 gauges are continuous during our study
 219 period, and the gauges with missing monthly datasets were spatially interpolated using the
 220 same technique from the GRACE data gaps. Table 1 details the information regarding the
 221 characteristics and source of the acquired datasets used in our study.

222 Table 1. Characteristics and sources of the dataset used in our processing.

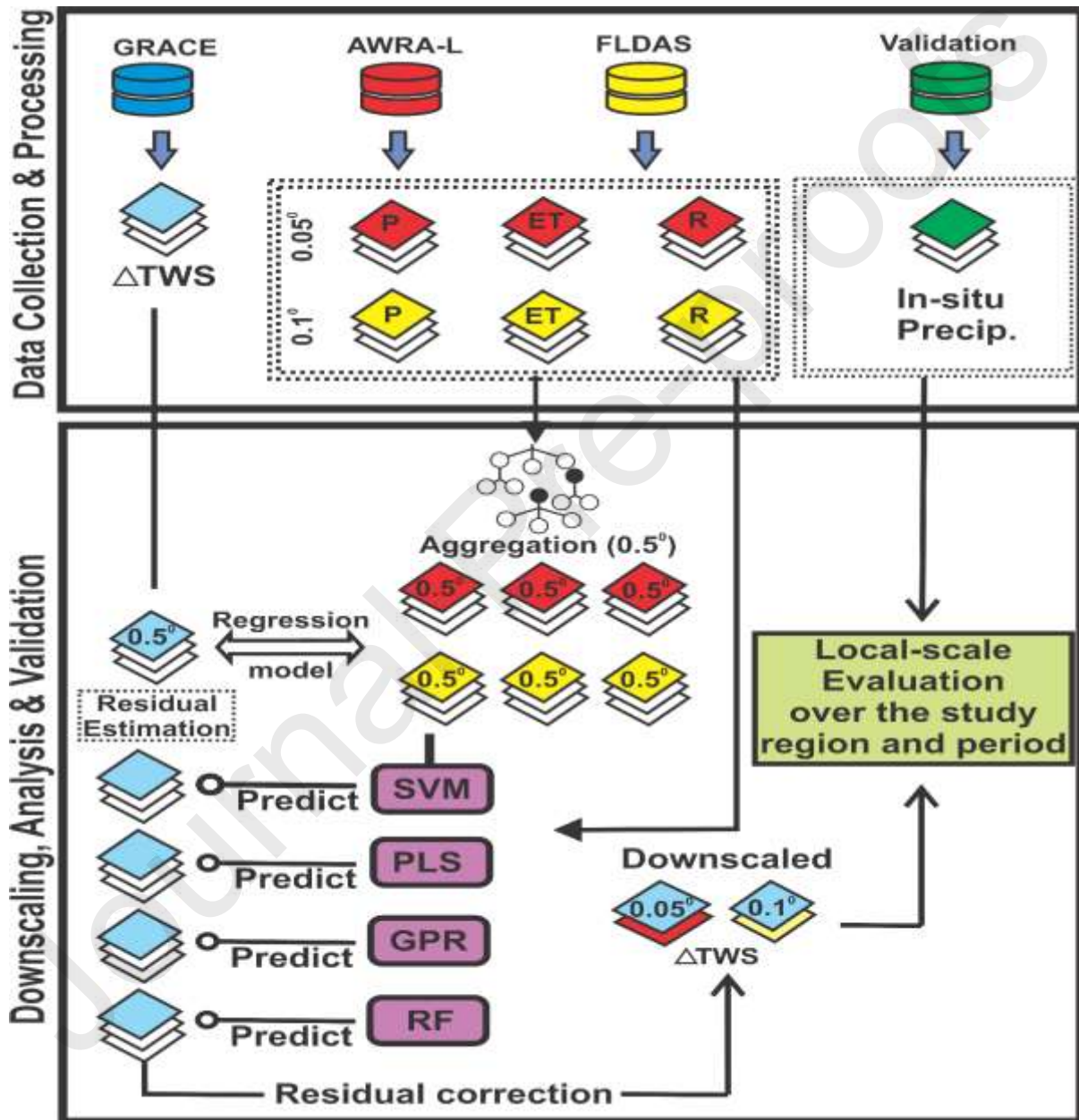
Type	Parameter	Mission	Resolution
Satellite (a)	Δ TWS	GRACE	$0.5^\circ \times 0.5^\circ$
Global Model (b)	Precipitation Evapotranspiration Runoff	FLDAS (Noah)	$0.1^\circ \times 0.1^\circ$
Regional Model (c)	Precipitation Evapotranspiration Runoff	AWRA-L (AWO)	$0.05^\circ \times 0.05^\circ$
In-situ (d)	Gauge precipitation	Observations	-

(a) https://www2.csr.utexas.edu/grace/RL06_mascons.html
 (b) https://disc.gsfc.nasa.gov/datasets/FLDAS_NOAH01_C_GL_M_001/summary?keywords=FLDAS_NOAH
 (c) <https://awo.bom.gov.au/products>
 (d) <http://www.bom.gov.au/climate/data/index.shtml>

224 **3. Methods**

225 3.1 Regression-based downscaling approach

226 A primary premise of the spatial downscaling method is that spatial relationships established
 227 between GRACE- Δ TWS and hydrological variables at a coarse spatial scale can be used for
 228 finer scale Δ TWS estimations using high-resolution predictors (Arshad et al., 2022; Khorrami
 229 et al., 2023). The specific steps of our regression-based downscaling approach are summarized
 230 in Fig. 2 and explained below.



231

232 Fig. 2. Schematic flow of the analysis used in this study.

233 i. *Data resampling and aggregation:* All high-resolution predictors from both models
 234 (precipitation, evapotranspiration, and runoff) were spatially resampled to coarse resolution of
 235 the original GRACE samples by pixel aggregation. This was necessary to achieve consistency
 236 in the spatial grain size of the predictors and response variables.

237 ii. *Machine learning*: Four different machine learning models (*see* section 3.2) were built to
 238 establish a regression-based relationship between the original GRACE-TWS and the predictors
 239 from the global and regional models, respectively. These models were used to predict TWS at
 240 0.5° .

241 iii. *Model residuals*: The predicted TWS was subtracted from the original GRACE TWS (0.5°
 242 $\times 0.5^\circ$) to obtain the model residuals for the respective learning models (ε).

243 iv. *Evaluation*: The predictive capabilities of each individual machine learning method was
 244 analysed and the residuals were subsequently interpolated to $0.10^\circ \times 0.10^\circ$ for the global and
 245 $0.05^\circ \times 0.05^\circ$ for the regional hydrological model predictors using ordinary kriging approach
 246 (Duan & Li, 2016; Arshad et al., 2022).

247 v. *Downscaling*: Downscaled Δ TWS estimates were obtained using high-resolution
 248 hydrological predictors from both global ($0.10^\circ \times 0.10^\circ$) and regional ($0.05^\circ \times 0.05^\circ$) models in
 249 conjunction with the residuals in step iv. The steps used in the prediction for each machine
 250 learning model are further detailed in section 3.2.

251 3.2 Machine learning models

252 In this study, we evaluated the capabilities of four different machine learning models in our
 253 regression-based downscaling, namely: support vector machines (SVM), partial least squares
 254 regression (PLR), gaussian process regression (GPR), and random forest (RF). Their
 255 formulations, statistical properties and how they were developed for our downscaling process
 256 are detailed below.

257 3.2.1 Support vector machines

258 The support vector machine (SVM) is a supervised learning technique proficient in linear and
 259 non-linear regressions. Its principle is based on the method of structural risk minimization and
 260 statistical learning theory (Kalu et al., 2023; Roy & Chakraborty, 2023). The SVM regression
 261 is considered a nonparametric technique because it relies on kernel functions. In SVM
 262 regression, the set of training data includes predictor variables and observed response values.
 263 The goal is to find a function $f(x)$ that deviates from y_n by a value no greater than ε for each
 264 training point x , and at the same time as flat as possible.

265 Suppose we have a set of training data where x_n is a multivariate set of N observations with
 266 observed response values y_n ; To find the linear function $f(x) = x'\beta + b$ and make sure it is as
 267 flat as possible, we must find $f(x)$ with the minimal norm value ($\beta'\beta$). This is expressed as a
 268 convex optimization problem to minimize $J(\beta) = 0.5 \times \beta'\beta$ subject to all residuals having a
 269 value less than ε (Vapnik, 1999)

270 It is possible that no such function $f(x)$ exists to satisfy these constraints for all points, which
 271 warrants the introduction of slack variables (ξ_i, ξ_i^*) for each point to deal with their respective
 272 infeasible constraints (eqn. S3-S4) (Smola & Schölkopf, 2004).

273 3.2.2 Partial least square regression

274 The partial least square regression (PLR) model is a two-edged multivariate tool as it combines
 275 features from multi linear regression and principal component analysis (Ndehedehe & Ferreira,
 276 2020). It decomposes the mean data of X (predictor variable) and Y (target variable) while

277 attempting to maximize the covariance between the two variables whilst complying with
278 certain normalization and orthogonality constraints (e.g., [Ndehedehe & Ferreira, 2020](#)).

279 Consider a set of data $\{(x_i, y_i); i = 1, 2, 3, \dots, n\}$, where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$, where n is the
280 number of samples (in our case 183). The centered data matrices X and Y are decomposed as

$$281 \quad X_{n \times p} = t_{n \times 1} P'_{p \times 1} + E_{n \times p}, Y_{n \times q} = u_{n \times 1} q'_{q \times 1} + F_{n \times q}, \quad (1)$$

282 where n is the corresponding dependent samples, t and u are latent vectors for the n
283 observations, p and q are the loading vectors, while E and F are the residual vectors. PLR
284 maximizes the square covariance between the latent vectors (t and u) to generate the projection
285 vectors w and h as $t=Xw$ and $u=Yh$ (see eqns. S7-S10) ([Yan et al., 2013](#); [Chen et al., 2018](#)).

286 3.2.3 Gaussian process regression

287 The Gaussian process regression (GPR) is a supervised non-parametric kernel-based
288 probabilistic model. It is a machine learning method based on the Bayes theory and statistical
289 learning theory ([Kalu et al., 2023](#)).

290 Consider a set of data $\{(x_i, y_i); i = 1, 2, 3, \dots, n\}$, where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$, drawn from an
291 indefinite distribution. The GPR algorithm attempts to predict the value of the target variable
292 y_{pred} based on a linear regression of the form

$$293 \quad y = x^T \beta + \varepsilon \quad (2)$$

294 where, $\varepsilon \sim N(0, \sigma^2)$. The priori distribution of the observation y and the joint prior distribution
295 of the observed y value and the predicted value, y_{pred} can be obtained by

$$296 \quad y \sim N(0, K(X, X) + \sigma_n^2 I_n) \quad (3)$$

$$297 \quad \begin{bmatrix} y \\ y_{pred} \end{bmatrix} \sim N \left(0, \begin{bmatrix} K(X, X) + \sigma_n^2 I_n & K(X, x_{pred}) \\ K(x_{pred}, X) & K(x_{pred}, x_{pred}) \end{bmatrix} \right) = N \left(0, \begin{bmatrix} K & K_*^T \\ K_* & K_{**} \end{bmatrix} \right) \quad (4)$$

298 where, $K(x, x)$ represents a symmetric positive definitive covariance matrix, whose elements
299 estimate the association between x_i and x_j through the chosen kernel function; $K(x_*, x) =$
300 $K(x_*, x)^T$ depicts the covariance matrix between the test sets, x_{pred} and the training set x ;
301 $K(x_*, x_*)$ depicts the covariance matrix of the test set itself; I_n represents an n -by- n unit matrix.

302 3.2.4 Random forest

303 Random forest (RF) integrates ensemble learning methods that combines multiple decision
304 trees to create a robust model. Each tree handles a subset of data to make a collective prediction
305 using bootstrapping for subsample selections, and randomness in decision making ([Heung et](#)
306 [al., 2014](#)). In RF regression, an extra function is utilized in combining the decision of individual
307 trees (Eqn. 5).

308 Consider a set of data for bootstrap aggregating $X = x_1, x_2, x_3 \dots x_n$ having a target of $Y =$
309 $y_1, y_2, y_3 \dots y_n$, the bagging of sub-sample repeated N times to fit the trees.

$$310 \quad \widehat{rF} = \frac{1}{N} \sum_{i=1}^N f_i(x') \quad (5)$$

311 where, $f_i(x')$ are the random forest trees and \widehat{rF} depicts the prediction of an unknown point x'
 312 using the bootstrapped dataset.

313 3.3 Evaluation metrics

314 The performance of our machine learning and downscaled products were evaluated using four
 315 statistical metrics which include spearman's rank correlation (R), Nash-Sutcliffe Efficiency
 316 (NSE), root mean square error (RMSE), and mean absolute error (MAE) (Rahman et al., 2023)
 317 (Eqns. S11-S14). It is important to point out that the use of original coarse GRACE data to
 318 validate the downscaled higher resolution data can be problematic. This is because the original
 319 GRACE data represents large scale regional trends, so it may not fully capture localized
 320 dynamics shown in the downscaled data. Therefore, the direct comparison to GRACE could
 321 underestimate errors in the downscaled products. To circumvent this, we performed a spatial
 322 aggregation of our downscaled products to allow for a direct comparison. We took spatial
 323 averages over larger areas closer to the GRACE resolution to provide a better and proficient
 324 method of consistency check. To further check for statistical inference, we resampled the
 325 downscaled products using bootstrapping. This process entails creating multiple simulated
 326 datasets for the SVM, PLR, GPR and RF algorithms by randomly sampling observations from
 327 the downscaled estimates with replacements. The simulated products were also used to estimate
 328 the properties of our statistical model and gauge the performance of our learning algorithms
 329 (Li et al., 2010; Arsenault et al., 2018).

330 3.4 Wavelet coherence

331 Wavelet coherence analysis is particularly well-suited for studying relationships between time
 332 series data that exhibit non-stationary and time-varying behaviour, making it a valuable tool
 333 for examining the association between hydrological variables. We used it to assess the local-
 334 scale evaluation of the various downscaled products (from different models and machine
 335 learning algorithms) over our test region and within the time-frequency space. Wavelet
 336 coherence attempts to determine the relationship between the variables (in-situ precipitation v.
 337 downscaled TWS) by estimating the correlation between them that varies between 0 and 1. The
 338 coefficient of wavelet coherence (Grinsted et al., 2004; Ali et al., 2022) between the two sets
 339 of time series can be denoted as

$$340 \quad R^2(s) = \frac{|S(s^{-1}W_n^{XY}(s))|^2}{s(s^{-1}|W_n^X(s)|^2) \cdot s(s^{-1}|W_n^Y(s)|^2)} \quad (6)$$

341 where $R^2(s)$ is the coherence coefficient minimum and maximum coherence at 0 and 1, and
 342 $W_n^{XY}(s)$ is the cross wavelet transforms between series two series (in our case, in-situ
 343 precipitation and all the downscaled TWS products), S is the smoothing operator and is
 344 represented as

$$345 \quad S(W) = S_{scale}(S_{time}(W_n(s))) \quad (7)$$

346 where, S_{scale} refers to smoothing along the wavelet scale axis and S_{time} smoothing in time.
 347 For our experiment, we examined the wavelet coherence at a 5% significance level.

348 To perform appropriate analysis and consider domain knowledge to interpret the underlying
 349 patterns of the in-situ precipitation and downscaled products, we transformed their time series
 350 into a series of percentiles. The transformed time series have been shown to react 'more
 351 linearly' to climate datasets (see Grinsted et al., 2004). The need to interpret the underlying

352 patterns more efficiently warranted our use of the continuous wavelet transform (CWT) to
353 extract a low signal-to-noise ration signal between the in-situ estimates and downscaled
354 GRACE-TWS. The CWT is a popular tool for assessing localized intermittent oscillations in
355 time series observations. However, it is mostly proficient in the examination of two time series
356 that are linked in some way. It can be very useful in investigating if regions in time frequency
357 intervals with large common power have a consistent phase interaction and suggests causality
358 between the time series observations.

359 3.5 Regression model and local scale evaluation/validation

360 The variables used for our predictions are representative of the dominant hydrological fluxes
361 of the region. Precipitation, evapotranspiration and runoff form the water budget equation
362 which illustrates the water exchange between the ocean, land and atmosphere. They
363 collectively regulate the movement, distribution, and availability of water within a region,
364 shaping its hydrological cycle and influencing both natural ecosystems and anthropogenic
365 activities.

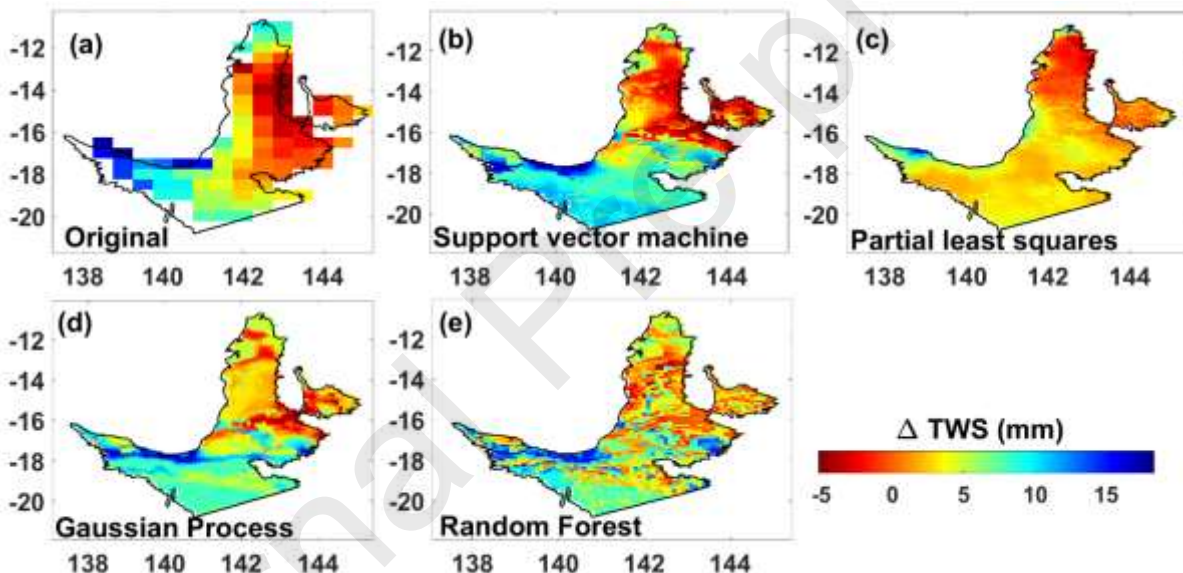
366 These variables and the GRACE-TWS were set as input and target variables, respectively for
367 each of the four algorithms explored in our experiment. The variables which were originally in
368 fine resolution were aggregated to the resolution of the GRACE-TWS to maintain consistency
369 between the spatial grains of the input and target variables. This enabled us to build a functional
370 regression model based on the four learning algorithms. These regression models were used to
371 predict GRACE-TWS both at the original scale and at a finer scale using the input variables at
372 their original resolutions. It was important to predict GRACE TWS at the original scale to
373 estimate the residuals between the observed and predicted GRACE TWS for each algorithm
374 and add them back to the predictions of the high-resolution GRACE TWS. Adding back the
375 residual after the entire downscaling process is a critical step to enhancing the accuracy and
376 spatial representation of the downscaled results. By incorporating residual information, the
377 downscaled estimates better capture finer-scale variability and localized features that are
378 important for understanding and managing terrestrial water storage dynamics at regional scales.
379 However, we attempted to evaluate the capabilities of the regression models in the prediction
380 of high resolution Δ TWS estimates based on the independent parameters of the regional and
381 global models before adding back the residuals. This is because the predicted values without
382 the residuals represent the systematic trends and relationships captured by the individual
383 learning models. By providing values based on the overall patterns and trends present in the
384 original GRACE data, we can efficiently gauge the performance of each learning model before
385 adding the residuals back to them.

386 One of the primary goals of statistical downscaling of GRACE-TWS is to provide more
387 detailed and localized information about changes in water storage within a specific region. It
388 therefore follows that the task of validating any downscaled product must be through a local-
389 scale hydrological metric. For our study, we validated our downscaled products and assessed
390 their closeness to local-scale hydrological variability using in-situ precipitation observations of
391 42 rain gauges scattered across our test region. In-situ precipitation observations provided
392 essential data to quantify rainfall input (which is regarded as the primary variable in the water
393 budget), model hydrological processes, validate models and manage water resources within a
394 catchment. Our choice of in-situ precipitation over satellite precipitation is aimed at assessing
395 information for accurate local-scale water storage assessments which has been observed to be
396 the most dominant contributor of GRACE- Δ TWS (Ndehedehe et al., 2021; Shah & Mishra,
397 2021; Kalu et al., 2022).

398 Finally, with the use of the bootstrapping resampling technique, we performed a probabilistic
 399 validation of the downscaled products against multiple simulated datasets which were
 400 randomly sampled from the respective regression models with replacement. This provided us
 401 the opportunity to carefully consider the uncertainty estimates of our regression-based
 402 downscaled products.

403 3.6 Global versus Regional model downscaling

404 GHMs ensure uniformity in modelling approaches and parameterization, which can be
 405 advantageous for comparative studies and global climate change analysis. This allows
 406 researchers to assess how changing climate patterns might affect water availability, distribution
 407 and related phenomena on a broad scale. We tried to understand how these numerous benefits
 408 of the GHM impacts on local-scale downscaling by using different regression-based algorithms
 409 (Fig. 3). And given that GHMs offer a reference point for evaluating the performance of
 410 regional models, comparing outputs from regional and global models could help identify areas
 411 where regional models exceed or provides a better characterization of local scale hydrology
 412 better than their global counterparts.



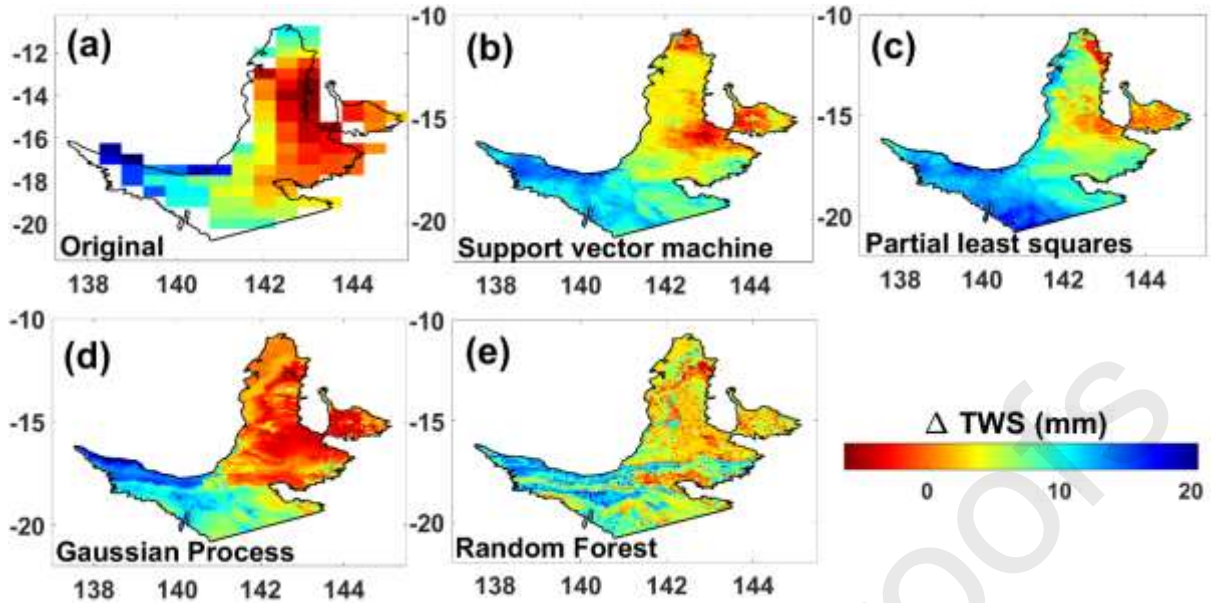
413

414 Fig 3. Regression-based downscaling at $0.1^\circ \times 0.1^\circ$ based on global hydrological models
 415 (FLDAS). These observations are the mean of monthly GRACE -TWS observations from April
 416 2002 to June 2017.

417 Surprisingly, we have more downscaling operations use GHMs than RHMs in their operations.
 418 Even though this may be due to the easy availability of GHMs, it is important to point out the
 419 relevance of RHMs in downscaling operations particularly in crucial areas with complex
 420 terrains, diverse land cover, or specific hydrological challenges.

421 We tested the same regression models used for the GHMs in RHMs (Fig. 4). This helped us to
 422 verify which hydrological model provides a more detailed assessment of local management
 423 practices on water resources.

424



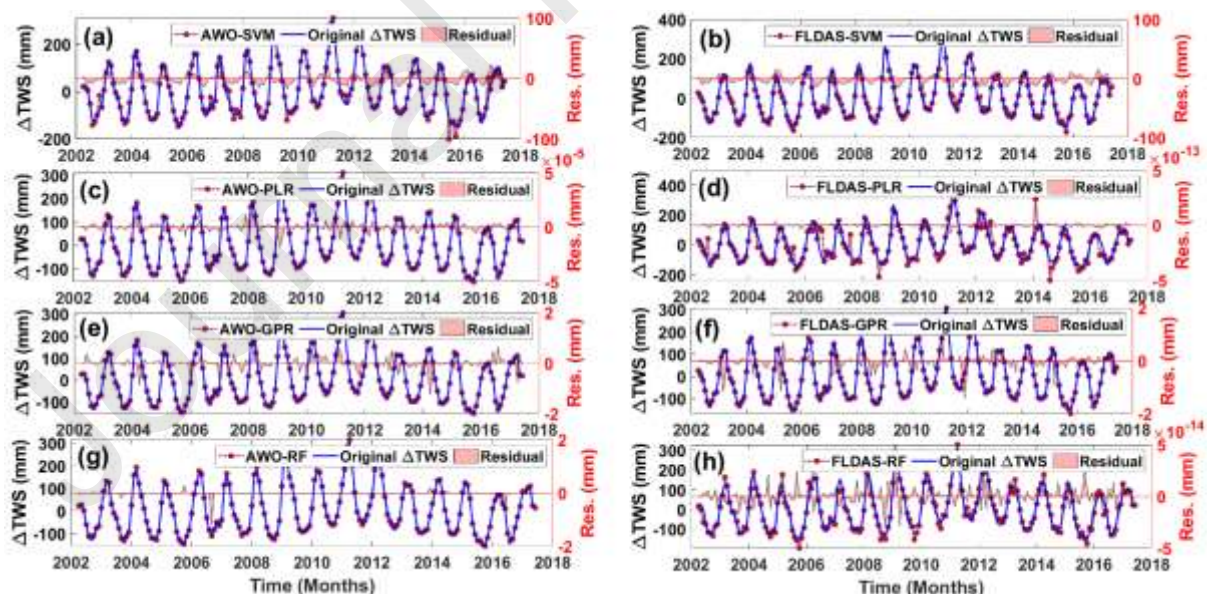
425

426 Fig 4. Regression-based downscaling at $0.05^\circ \times 0.05^\circ$ based on regional hydrological (AWO)
 427 models. These observations are the mean of monthly GRACE -TWS observations from April
 428 2002 to June 2017.

429 4. Results and Discussion

430 4.1 Performance of the regression models

431 To gauge the performance of the regression models, it was necessary to compare the original
 432 and downscaled ΔTWS estimates (Figs. 5, 6).



433

434 Fig 5. Time series of the original and downscaled GRACE-TWS for each algorithm before
 435 adding back the residuals. The regional and global hydrological models which are represented
 436 in panels a,c,e,g and b,d,f,h, respectively, are used to downscale GRACE TWS. The right
 437 ordinate (coloured red) in each pane represents the residuals which depicts the differences
 438 between the original and predicted values.

439 For the regional based predictions, the gaussian process regression showed exceptionally high
 440 agreement ($R = 0.99$, $NSE = 0.99$), and the lowest MAE (0.80mm) and RMSE (1.44mm),
 441 respectively. This is followed by the partial least square regression model with MAE (1.22mm)
 442 and RMSE (1.77mm) slightly higher than the gaussian process regression model. The random
 443 forest also maintained a very good fit with MAE and RMSE values of 3.58mm and 4.80mm,
 444 respectively, while the support vector machine, which provided a very good fitting of ($R =$
 445 0.98 , $NSE = 0.97$, $RMSE = 17.04$ mm, and $MAE = 10.67$ mm) has the lowest fitting amongst
 446 the four models used for the regional-based predictions (Fig 6a-d). The global based predictions
 447 tended to be slightly less accurate than the regional based predictions. The gaussian process
 448 regression also indicated the highest agreement between original and downscaled products ($R =$
 449 0.99 , $NSE 0.99$), and the lowest MAE (4.63mm) and RMSE (7.20mm), respectively. The
 450 support vector machine also showed considerably strong agreement ($R = 0.98$, $NSE = 0.97$),
 451 with MAE and RMSE values of 12.11mm 15.49mm, respectively. The random forest
 452 regression model also produced a good fitting index of R (0.98mm), NSE (0.95), MAE
 453 (17.72mm) and RMSE (23.69mm), while the partial least square regression had the lowest
 454 fitting index of R (0.91), NSE (0.81), MAE (26.79mm) and RMSE (44.71mm) amongst the
 455 four models used for the global-based predictions (Fig. 6e-h). The varied performance of these
 456 learning algorithms under different scenarios (regional and global predictors) shows that the
 457 inherent differences between the regional and global datasets significantly impacts on the
 458 performance and behaviour of the machine learning models and hydrological model properties
 459 such as data distribution, scale discrepancy and spatial variability are key in maintaining
 460 accuracy and consistency in regression models.

461 Overall, the downscaled results were consistent with the original GRACE- Δ TWS observations
 462 (Fig. 5). Finer spatial patterns were discernible with the increased spatial resolution for all the
 463 machine learning methods compared to the original GRACE- Δ TWS observations (Fig. 3 and
 464 4). We however observed an increase in the range between the maximum and minimum
 465 downscaled values with the regional-based downscaled TWS values having a wider range
 466 (Table 2). On average, the range of all the downscaled estimates increased slightly (Table 2),
 467 thereby widening the contrast between the data and the highlighting spatial patterns.

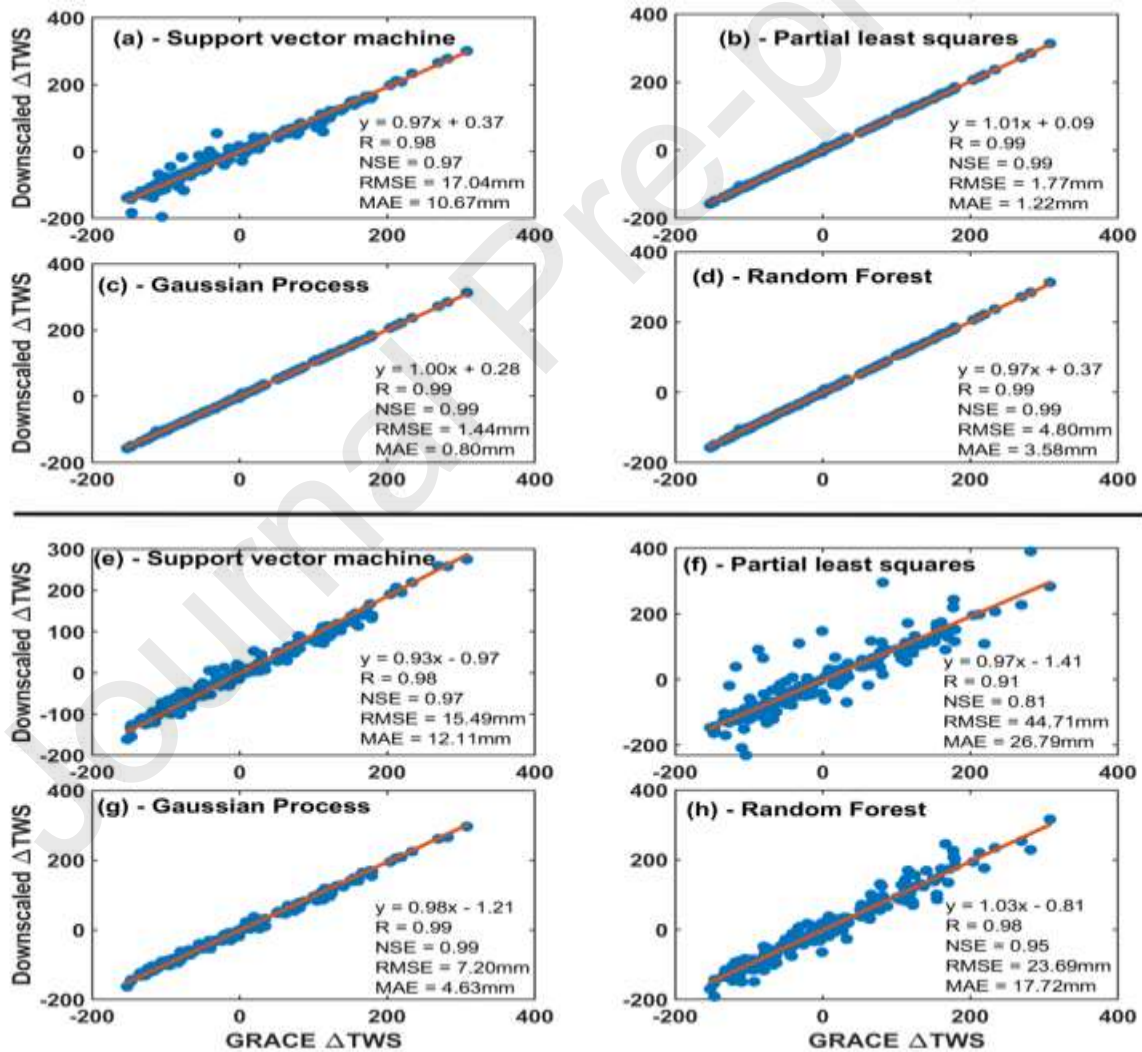
468 Table 2. summary attributes of the original and downscaled Δ TWS estimates

Δ TWS	Min (mm)	Max (mm)	Average (mm)	SD (mm)	CV (unitless)
GRACE-CSR	-196.17	328.20	4.81	108.56	18.84
AWO-SVM	-202.29	311.31	5.66	101.02	17.85
AWO-PLR	-155.83	310.14	5.61	104.05	18.56
AWO-GPR	-153.62	308.13	5.72	103.47	18.09

AWO-RF	-156.67	314.73	6.21	104.64	16.86
FLDAS-SVM	-171.54	295.49	4.15	97.42	23.49
FLDAS-PLR	-237.58	405.01	3.89	109.39	28.15
FLDAS-GPR	-167.21	305.50	4.27	101.43	23.77
FLDAS-RF	-196.17	328.20	4.81	108.56	22.55

469 Note: SD = Standard deviation, CV = coefficient of variation

470



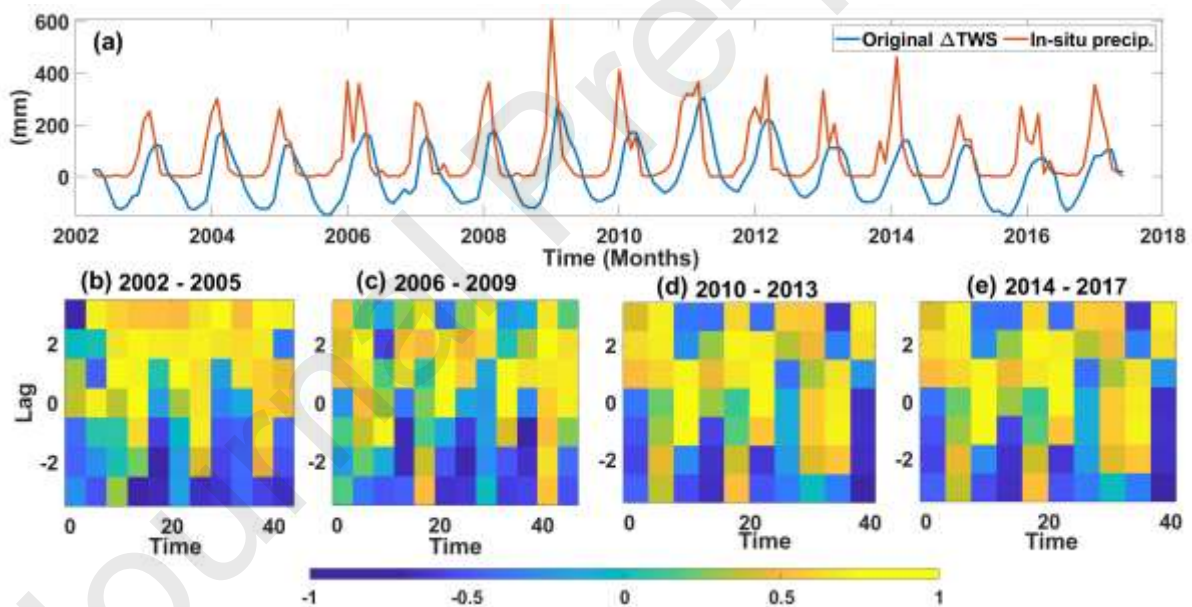
471

472 Fig 6. Accuracy estimation of the machine learning models after adding the residuals back to
 473 the high-res. predictions. The upper panel (a - d) represents regional based predictions from the
 474 AWO, while the lower panel (e - h) represents global based predictions from the FLDAS model.

475 The x-axis shows the TWS derived from GRACE and the y-axis shows the downscaled TWS
 476 from the four machine learning methods for both regional (Fig. 6a-d) and global (Fig. 6e-f)
 477 based variables.

478 4.2 Validation and local-scale assessments

479 Precipitation plays a key role in driving terrestrial water storage by providing the primary
 480 source of water that replenishes various reservoirs within the earth's hydrological cycle
 481 (Khandu et al., 2016; Fatolazadeh & Goïta, 2021). When precipitation occurs, it infiltrates the
 482 soil, replenishing soil moisture and groundwater reservoirs. Additionally, it contributes to the
 483 filling of lakes, rivers, and other surface water bodies. Therefore, monitoring precipitation
 484 patterns is essential for understanding the availability and distribution of water resources in a
 485 region as they tell the most relatable story about the water storage dynamics in a localized unit.
 486 This is also evidenced in their action as the key variable in the water budget equation (Lehmann
 487 et al., 2022) in comparison to the other hydrological flux variables (ET and runoff). Their role
 488 in driving localized water storage dynamics is depicted in the strong relationship noticed
 489 between TWS and precipitation as shown in Figure 7a. Their relationship, however, is affected
 490 by lags which vary for different regions. We observed a two-month lag between precipitation
 491 and TWS for our entire study period which was partitioned into a four-year epoch (Fig. 7b, c,
 492 d, e) for a more detailed assessment. Our partitioning shows that the 2-month lag experienced
 493 over our study period was more consistent and strongest between 2002 to 2005 (Fig. 7b).



494

495 Fig 7. Windowed cross correlation between monthly precipitation and TWS signals up to a pre-
 496 defined lag of 3 months. Precipitation drives terrestrial water storage and therefore provides a
 497 key metric (via in-situ observations) for local scale water storage assessments. The lag between
 498 precipitation and TWS was assessed over four-year epochs (Figs. 7b, c, d, e) partitioned from
 499 the study period. The warm yellow grids represent a lag of $> +2$ months while the cool blue
 500 grids represent a lag of < -2 months.

501 It is important to point out that lag effects between precipitation and TWS are affected by
 502 factors such as varying soil types, land cover, geological characteristics etc. The CB which is
 503 characterized by a mix of sediments, sands, clays and gravels witnesses a diffuse percolation
 504 of precipitation as the soil is often porous, thereby allowing rainwater to infiltrate the ground.

505 This helped to ensure the minimum lag period of two months between precipitation and
 506 terrestrial water storage as is the case with other regions having similar hydrogeological
 507 frameworks (e.g., Ndehedehe & Ferreira, 2020; Kalu et al., 2021). The heterogenous nature of
 508 the hydrogeological formation of the CB results in the varying percolation rates in different
 509 parts of the basin which translates to inconsistent lag period between precipitation and TWS as
 510 shown in figure 7. The most inconsistent lag period was recorded between 2006 to 2009 (Fig.
 511 7c). This may not be totally unrelated to the heavy rains in 2009 and 2010 that terminated the
 512 Australian millennium drought which started in 1997 (Ndehedehe, 2022b), thus disrupting the
 513 10-year drought-induced hydrological cycle. This shows that the highly variable nature of
 514 precipitation in time and space gives us the best representation of terrestrial water storage
 515 dynamics over all scales.

516 4.2.1 Hydrological flux variable (In-situ precipitation) as a metric for local-scale water
 517 assessments

518 In-situ precipitation datasets was used as an index for local-scale water assessments by
 519 observing the similarity in trend between the time series of the in-situ precipitation and the
 520 GRACE TWS datasets over our study period (Fig. 7). This also provided another avenue to test
 521 which of the machine learning models best mimics the trend. This is important because it is
 522 expected that the downscaled estimates should represent regional scale features and trends not
 523 present in the original estimates. Between April 2002 and July 2017, the difference between
 524 the long-term linear trends of the in-situ precipitation. and GRACE TWS was +0.09mm/month,
 525 where each had a positive trend of +1.36 and +1.45, respectively. The GPR and the RF for both
 526 the regional and global datasets best captured these trends in both short and long term (Table
 527 3). The linear trends of the different downscaled products and the in-situ precipitation values
 528 are summarized in Table 3.

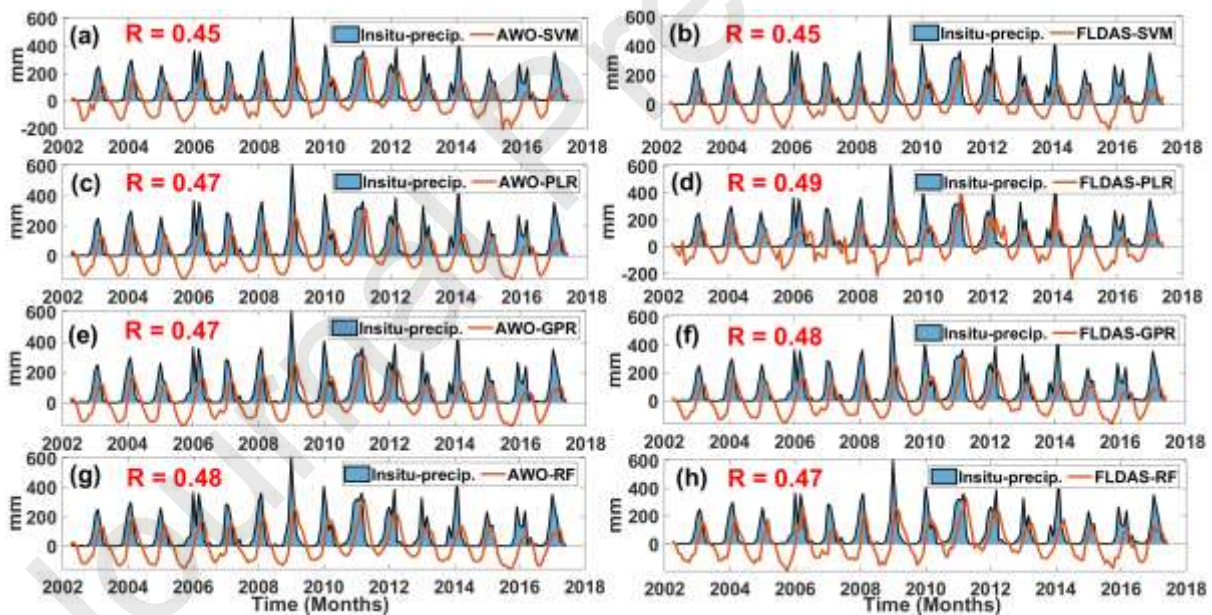
529 Table 3. Comparison of in-situ precipitation and Δ TWS linear trends at different spatial
 530 resolutions over our test region. The rain gauges depict the localized hydrological patterns,
 531 while the GRACE-CSR, FLDAS and AWO models represents the satellite, global-downscaled
 532 and regional-downscaled Δ TWS estimates whose trends are evaluated against the in-situ
 533 precipitation patterns.

Resolution	Precip. / Δ TWS	Data Source	Trend (mm/month)		
			2002 - 2009	2010 - 2017	2002 - 2017
-	Rain gauges	In-situ	+5.35	-7.72	+1.36
0.5°	GRACE-CSR	Satellite	+4.07	-14.92	+1.45
0.1°	FLDAS-SVM	Global model	0.00	0.00	0.00
	FLDAS-PLR		0.00	0.00	0.00
	FLDAS-GPR		+3.94	-15	+1.71
	FLDAS-RF		+3.51	-16.02	+2.18

0.05°	AWO-SVM	Regional model	0.00	0.00	0.00
	AWO-PLR		0.00	0.00	0.00
	AWO-GPR		+4.00	-14.83	+1.44
	AWO-RF		+3.85	-14.96	+1.33

534

535 Figure 8 demonstrates the correlation between the averaged in-situ precipitation gauges and all
 536 the regression-based variants of the downscaled GRACE-TWS for both regional and global
 537 hydrological models. it is important to note that the in-situ precipitation observations used in
 538 this exercise were heterogeneously distributed with most readings coming from the lower
 539 regions. However, they maintained reasonable uncertainty and deemed suitable for our analysis
 540 (Table S1). The global model prediction of the partial least square regression (Fig 8d)
 541 maintained the strongest correlation between the downscaled and in-situ precipitation
 542 observations. Overall, we observed that the signals of the global hydrological models
 543 performed slightly better than those of the regional hydrological models in characterizing local-
 544 scale water storage changes by their higher correlations with the in-situ estimates (Fig. 8b, d
 545 ,f).

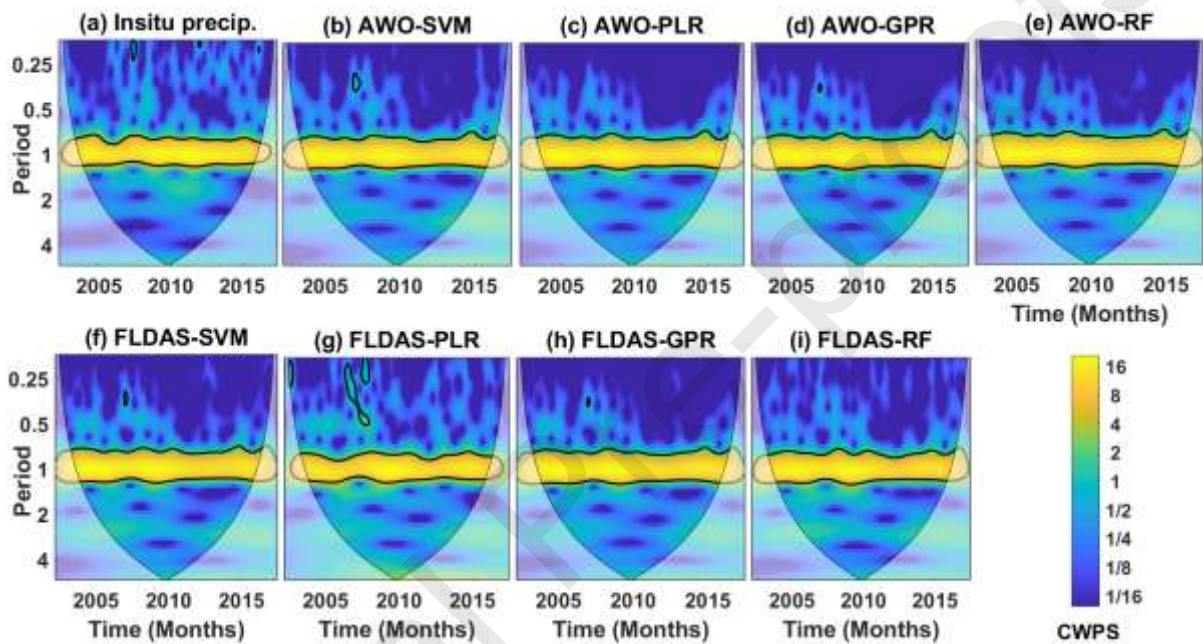


546

547 Fig 8. Raw assessment of the collinearity between the downscaled products and the in-situ
 548 estimates used for our local-scale assessment. Figures a, c, e, g and b, d, f, h represents the
 549 relationship between the in-situ precipitation patterns and the downscaled products from the
 550 regional and global hydrological models, respectively.

551 To better understand the signals at different spatial scales, we utilized the CWPS in identifying
 552 the contributions of short- and long-term fluctuations in the time series of the in-situ
 553 precipitation and downscaled estimates. The power is given by the colour. The colour ranges
 554 from blue (low power) to yellow (high power). The yellow colours represent areas of high
 555 power. Figure 9 provides insight to the time-frequency content of the in-situ precipitation

556 estimates and all the downscaled products at a 5% confidence level. Our result captured a
 557 dominant frequency band corresponding to seasonal cycles, semi-annual oscillations, and even
 558 shorter-term variations. For example, a noticeable power spike in 2006 is noticed in the CWPS
 559 plot for precipitation (Fig. 9a), and the downscaled product that best mimicked this spike was
 560 the FLDAS-PLR (Fig. 9g). This agrees with the result in Fig 8d where the PLR produced the
 561 strongest correlation with the in-situ precipitation estimates. The high frequency power spike
 562 noticed in Fig. 9a is representative of climate actions (such as El Nino Southern Oscillation -
 563 ENSO) in regulating precipitation patterns. The spikes noticed in the downscaled products (Fig.
 564 9b-i) are often linked to extreme weather events, such as intense rainfall or drought and the
 565 CWPS technique provides a robust way to detect such events and study their frequency
 566 characteristics.

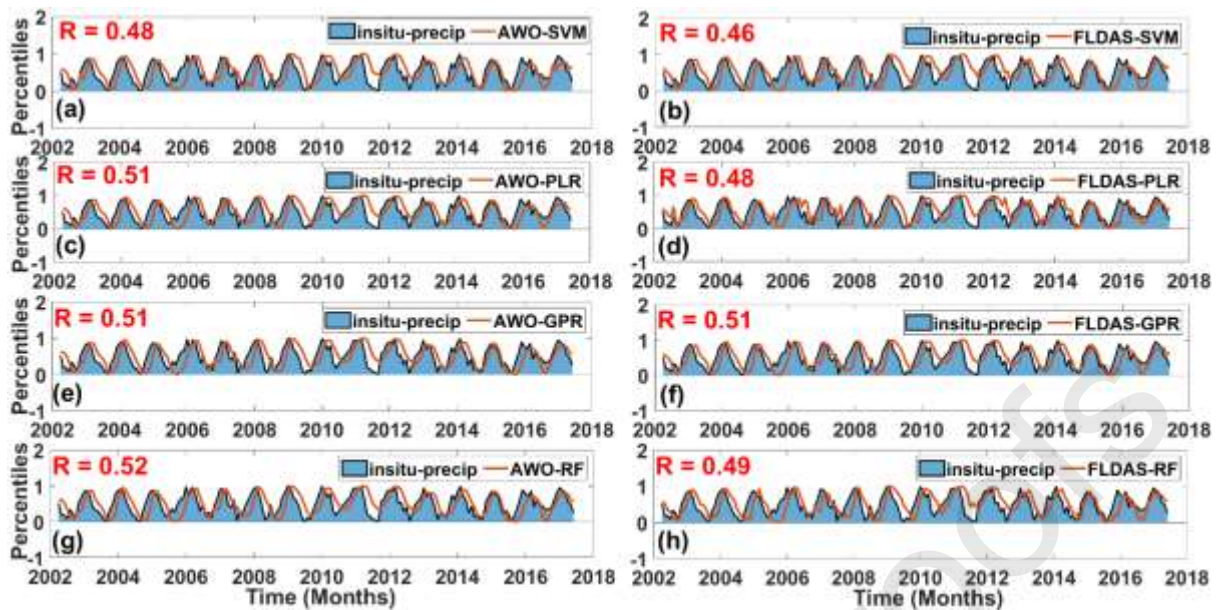


567

568 Fig 9. The continuous wavelet power spectrum of the in-situ observations (a), regional-based
 569 downscaled estimates (b - e) and the global-based downscaled estimates (f - i). The thick black
 570 contour represents the 5% significance level against the noise and cone of influence. NB:
 571 CWPS means continuous wavelet power spectrum.

572 4.2.2 Local scale examination and uncertainty assessment of the downscaled products

573 The local scale examination of the downscaled products is important to depict which
 574 hydrological model best characterizes the hydrology of small catchments. This examination
 575 was done by investigating the connection and relationship between the standardized time series
 576 in the light of the expected causality links.



577

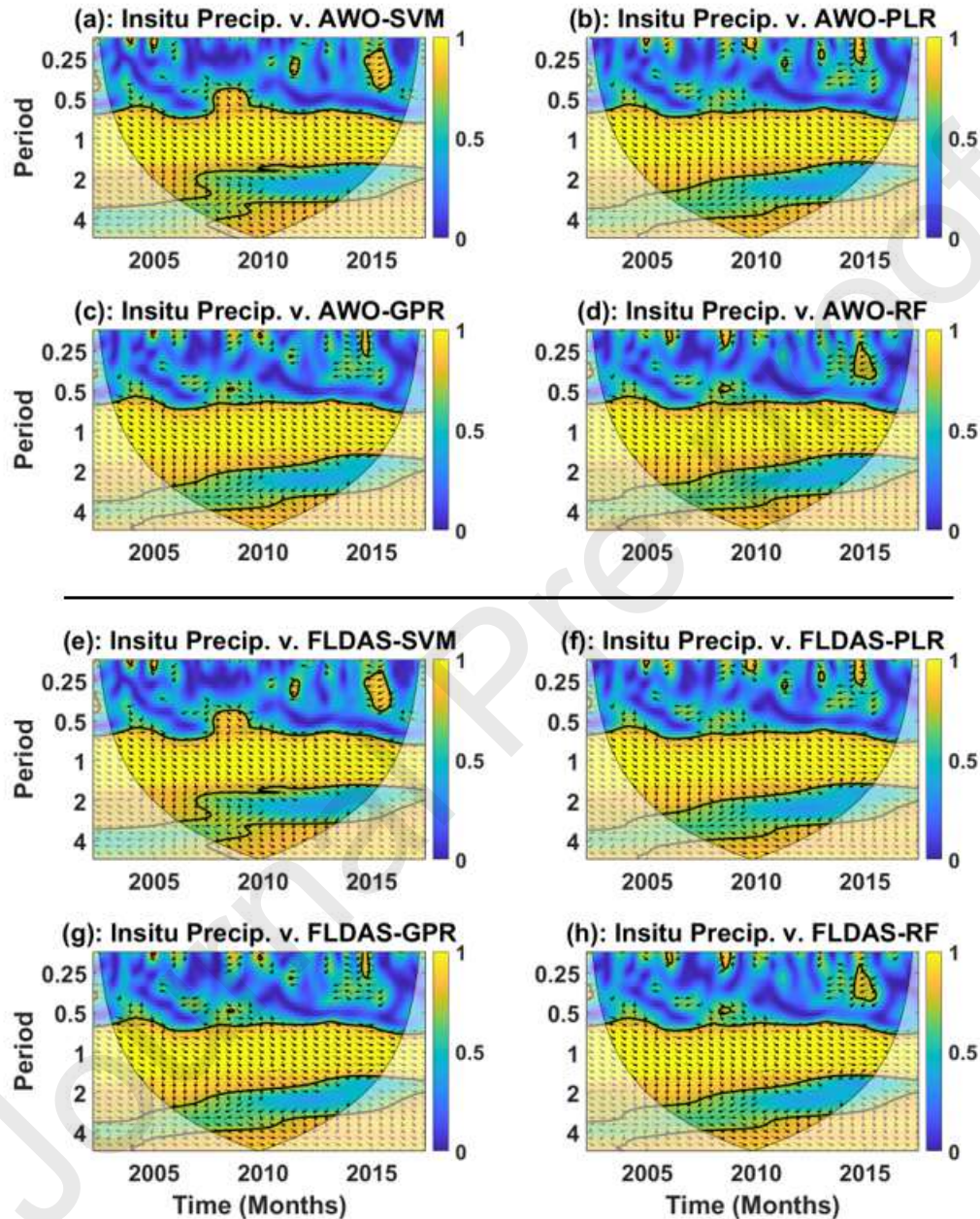
578 Fig 10. The standardized time series of in-situ precipitation and the region-based (a,c,e,g) and
 579 global-based (b,d,f,h) downscaled products. The time series have been transformed into a series
 580 of percentiles as shown in the y-axis.

581 We observed a stronger correlation between the standardized in-situ observations and the
 582 downscaled products in Fig. 10 than we did in the raw time series in Fig 8. The standardization
 583 shown in Fig 10 was achieved by transforming the probability density function (pdf) of the
 584 time series observations into a record of percentiles (in terms of its cumulative distribution
 585 function) thus forcing the pdf to be rectangular. This has the impact of limiting the width of
 586 intermittent oscillations and enhancing model fitting and improving predictive accuracy. The
 587 time series observations in Fig. 10 reveals patterns, trends and relationships which were not
 588 evident in the time series of Fig 8. Results from the transformed datasets revealed that for the
 589 region-based downscaling, the random forest prediction produced the best fitting with $R=0.52$
 590 (Fig. 10g). The gaussian process and partial least squares regression both produced a good
 591 fitting index of 0.51, while the support vector machine produced a fitting index of $R = 0.48$.
 592 Whereas, for the global-based downscaling, the gaussian process regression produced the best
 593 fitting with $R=0.51$ followed by the random forest regression, partial least squares regression
 594 and the support vector machines with R values of 0.49, 0.48, and 0.46, respectively. This result
 595 is in line with accuracy estimation of the machine learning models shown in Fig. 6.

596 Our experiment therefore shows that region-based predictors represent a better characterization
 597 and depiction of large-scale hydrological dynamics over their global counterparts. This was
 598 further represented in the wavelet coherence plot in Fig. 11. Regions are evident in the time
 599 frequency domain depicted in Fig. 11 where the in-situ precipitation and the downscaled time
 600 series co-vary but may not necessarily have high power (Adeyeri & Ishola, 2021). The hot
 601 colours (yellow) depict regions with a significant coherence, while the cooler colours (blue)
 602 represent a lesser degree of coherence between the in-situ precipitation and downscaled
 603 estimates. High-frequency powers of 0.8 and 1 are pronounced over the entire plots showing a
 604 significant relationship between the standardized precipitation and downscaled TWS series.
 605 The span of their periodicities varies for the various machine learning models. It is important
 606 to point out that the area of a time frequency plot above the 5% significance level is not an
 607 accurate depiction of causality. Even if the scales have been correctly weighted for the
 608 averaging, it is still a possibility that the in-situ precipitation and the corresponding downscaled

609 estimate be perfectly correlated at a particular scale while the area of significant correlation is
 610 less than the 5% significance level. Notwithstanding, our results from Fig. 11 suggests that the
 611 in-situ precipitation mirrors the corresponding downscaled products which means that our
 612 significance level is extensive and suitable for our experiment.

613

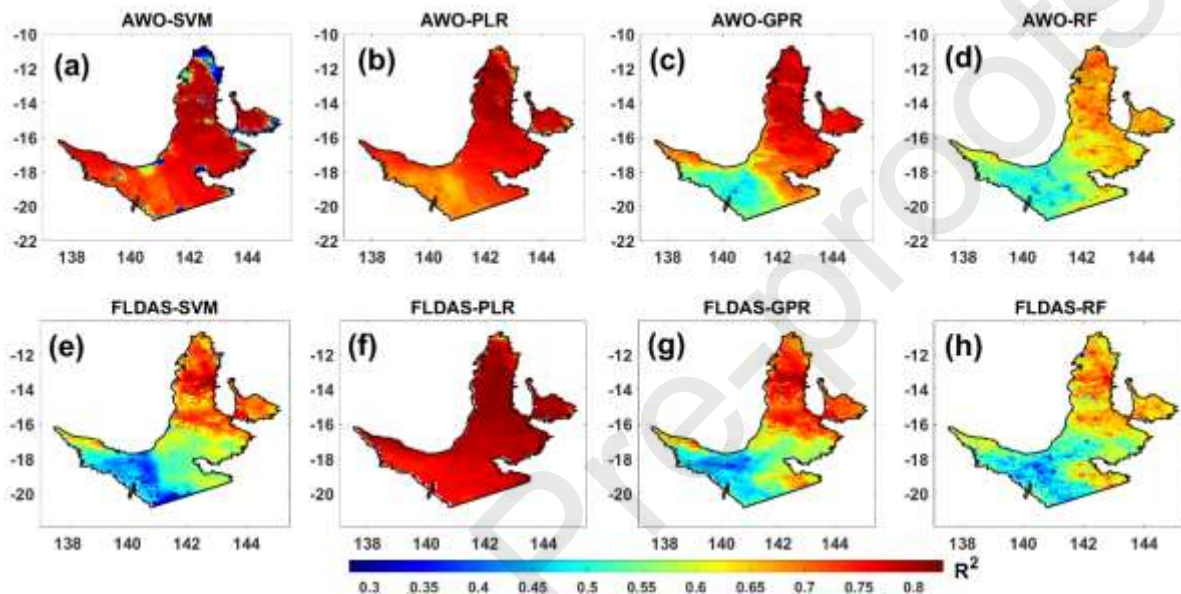


614

615 Fig 11. Squared wavelet coherence between the standardized estimates of the insitu
 616 precipitation and the region-based (a-d) and global-based (e-h) downscaled products. The 5%
 617 significance level against the noise is shown as the polygon contours.

618 For the regional based models, the SVM showed relatively high uncertainties towards the
 619 northern part of the test region (Fig. 12a). These uncertainties are attributed to the strong
 620 influence and processes of multi-annual water storage which has been documented to be
 621 prevalent in the area (Kaushik et al., 2021). These processes have resulted to complex

622 properties of the CB as it relates to exchange of fluxes and water storage. For the global based
 623 models, the SVM showed a relatively low R^2 value towards its western end, and this scenario
 624 was consistent in the GPR and RF algorithms for both regional and global hydrological models
 625 (Fig. 12c, d, e, g, h). These low R^2 values could imply strong interactions with non-climatic
 626 factors such as land-use and anthropogenic influences. Another plausible explanation could be
 627 that the regression models (i.e., SVM, GPR and RF) are not suitable for modelling the location
 628 unlike the partial least square regression (Fig. 12b, f) which maintained a strong R^2 value across
 629 the entire test region for both regional and global hydrological models. Overall, the four
 630 regression models show a good fit and can be relied upon for the statistical downscaling
 631 operation of hydrologically dynamic regions.

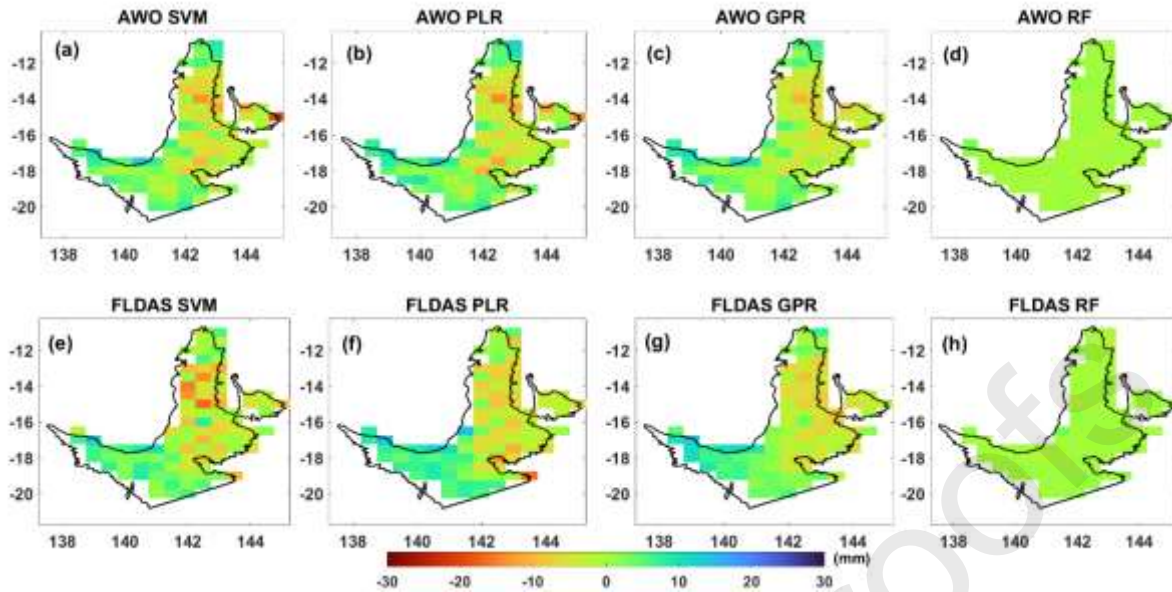


632

633 Fig 12. Uncertainty assessment of the downscaled products using bootstrapping. Areas of
 634 relatively high uncertainty correspond with lower R^2 values and vice versa.

635 4.2.3 Residual correction

636 Residual correction is an important step in statistical downscaling operations. Its primary
 637 purpose is to account for finer-scale variations that the initial downscaling model (i.e., predicted
 638 TWS at high resolution) may not capture (Fig. 13). Even though the initial downscaling process
 639 aims to improve the representation of regional-scale features, it is still composed of large-scale
 640 patterns which may not clearly depict fine-scale details of the downscaled product. However,
 641 adding back residuals fine-tunes the downscaled estimates by adjusting for unmodeled fine-
 642 scale variability and ensures that the final downscaled datasets represents both the regional and
 643 local conditions accurately.



644

645 Fig 13. Spatial representation of the residuals between the original and predicted GRACE TWS
 646 estimates for the SVM (a,e), PLR (b,f), GPR (c,g), and RF (d,h) machine learning models
 647 applied in our study. These residuals account for the complex variabilities that may not be
 648 captured in the downscaling operation and must be added back to the predictions to correct
 649 systematic bias and ensure a more realistic representation of our downscaled products.

650 The relatively high uncertainties observed in the SVM model (Fig. 12a, e) is made more distinct
 651 in Fig. 13a,e showing that the SVM was not able to effectively capture the complex
 652 hydrological variabilities exhibited in the study region. The GPR and RF methods had the least
 653 residuals across the entire study region for both regional and global models which resulted in
 654 the relatively high accuracy achieved in their downscaling and machine learning predictions
 655 processes (Fig. 5, 6). This shows that the probabilistic predictions and ensemble learning
 656 method of the GPR and RF, respectively, are effective in the modelling and capturing of
 657 complex hydrological signals evident in the CB compared to other machine learning methods.

658 4.3 Limitations and future directions

659 Results from our analysis may be affected due to the different sources of uncertainties involved.
 660 One of them lie in the inherent processing errors of the original GRACE estimates which was
 661 circumvented using mascon solution data, which appears superior to the spherical harmonics
 662 data (Aryal & Zhu, 2020; Khorrami et al., 2023). Moreover, our technique of filling the missing
 663 monthly data gaps using a linear interpolation approach may induce the associated uncertainties
 664 of the GRACE data considering the non-linearity of climate datasets. But given its ease in
 665 application and prevalent utilization within the hydrologic community, we reconstructed the
 666 missing months using a linear interpolation method. Another issue applies to the uncertainties
 667 of the global and regional hydrological models used to extract high-resolution predictors for
 668 our downscaling operation (Table S1). Cao et al. (2015) suggests that a key solution in
 669 diminishing the uncertainties posed by hydrological model outputs is to use the ensemble mean
 670 of several models with the same characteristics. However, due to the lack of many hydrological
 671 models simulated at 0.1° and 0.05° spatial resolution for the global and regional models,
 672 respectively, we only applied the FLDAS and AWO datasets in this current study.

673 Another issue lies in the interpolation of the residuals to match the spatial grain size of the
674 high-resolution predictors. Examination of residual in statistical downscaling operations help
675 bridge the gap between large-scale climate model outputs and fine-scale observations, capture
676 local variability, maintain statistical relationships, and provide a means for uncertainty
677 assessments. It is important we explore more technical capabilities besides interpolation in
678 treating these residuals as their inclusion to the predicted components ensures accuracy,
679 consistency and makes the downscaled values representative of the original observations.

680 It is important to note that climate actions and anthropogenic influences could introduce further
681 uncertainties to the local-scale assessments of downscaled products. This is due to factors such
682 as urbanization and land-use changes which could easily introduce biases into in-situ
683 precipitation measurements resulting to a modification of local precipitation patterns which
684 may not reflect the true water storage changes of the test region. Therefore, for other
685 experiments that wish to replicate our study, it is important to account for these influences,
686 consider data quality and representativeness, and assess the broader implications of human-
687 induced changes on the hydrological cycle of the test region.

688 **5. Conclusions**

689 The core of downscaling operations lies in the assimilation of additional high-resolution
690 information to improve the estimates of the target variable in the characterization of catchment-
691 scale operations. The task of downscaling is important because water decision makers and
692 managers are usually concerned with water storage changes at scales much smaller than the
693 resolution of GRACE data. It follows therefore that, to realize the full potential of GRACE in
694 hydrology, monthly GRACE-TWS should be downscaled to meet the requirements of local-
695 scale water resource management. This study explored two sets of high-resolution predictors
696 from global (FLDAS) and regional (AWO) hydrological models to downscale GRACE-TWS.
697 Our choice of the different model types was to ascertain which gives a better assessment of
698 hydrological dynamics on a local scale. To achieve this, we validated the downscaled products
699 with in-situ precipitation datasets scatter across the test region. The validation assessment
700 provided insights to which hydrological model best characterizes the dynamics of local-scale
701 hydrology as well as the method. We explored four different machine learning methods in our
702 downscaling operation and tested their prediction capabilities on both models.

703 The machine learning methods (SVM, PLR, GPR, RF) are used to downscale GRACE-TWS
704 using a regression-based approach from the spatial resolution of 0.5° to 0.1° and 0.05° for the
705 global and regional hydrological model estimates, respectively. It was important to measure
706 how well each regression model performed in (i) establishing a functional regression model
707 between predicted and observed TWS estimates, and (ii) predicting high resolution GRACE
708 TWS using the model parameters. To achieve this, we gauged the performance of each learning
709 using statistical metrics prior to adding back the residuals. This was warranted because the
710 predicted values without the residuals represent the systematic trend and relationships captured
711 by the individual learning models and provides a framework to gauge their unalloyed
712 performances. The GPR made the best prediction across board with RMSE and MAE values
713 of 1.44mm, 0.80mm for the regional model and 7.20mm, 4.63mm for the global model
714 estimates. This gives credence to the probabilistic framework of the GPR in model data
715 assessments and its ability to capture spatial correlations and temporal dependencies prominent
716 in hydrological datasets.

717 Overall, the findings of our study reports that the region-based downscaled TWS using the
718 random forest method provided the best characterization of local scale hydrology over our test

719 region. This was because it maintained the most significant correlation to the in-situ
 720 precipitation values. To get the most out of this relationship, we transformed the probability
 721 density function of the time series for the in-situ precipitation and all the downscaled estimates
 722 into a record of percentiles. This helped force the pdf into a rectangular form thus limiting the
 723 impact of intermittent oscillations dominant in hydrological variables and improving their
 724 respective predictive accuracies. Another advantage of this operation is that it has not outliers.
 725 Generally, our downscaling algorithm is efficient and reliable over out test region, where the
 726 primary assumptions were satisfied. This low-cost approach provides insights to which model
 727 and method best suits downscaling over regions with significant hydrological dynamics. This
 728 study basically focused on the technique and datasets used for statistical downscaling, and the
 729 use of a more robust, continuous and comprehensive in-situ precipitation network can be
 730 further investigated to combat the biases posed by land-use changes and urbanization in the
 731 validation of local-scale water resources in future research.

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- 902
- 903 • RHMs better characterizes the dynamics of local scale hydrology more than GHMs
 904 • Probabilistic framework of the GPR improves its ability in hydrological modelling.
 905 • In-situ precip. provides a key metric for local-scale water storage assessments.
 906 • Regression downscaling effectively enhances GRACE-TWS res. for local evaluations

907

908 CRedit authorship contribution statement

909 **Ikechukwu Kalu:** Writing – original draft, Writing – review & editing,
 910 Methodology, Formal analysis, Conceptualization, Investigation,
 911 Software. **Christopher E. Ndehedehe:** Conceptualization, Supervision, Software,
 912 Investigation, Formal analysis, Methodology, Writing – original draft, Writing –

913 review & editing. **Vagner G. Ferreira:** Supervision, Writing – original draft,
914 Writing – review & editing, Formal analysis. **Mark J. Kennard:** Conceptualization,
915 Supervision, Software, Writing – review & editing.

916

917

918 **Abstract**

919 The coarse spatial resolution of the Gravity Recovery and Climate Experiment (GRACE) data
920 has limited its application in the management of local-scale water resources. To address this
921 limitation, we developed a new downscaling approach using predictors from regional and
922 global hydrological models for a 15-year period (2002-2017) and tested it in the northern Great
923 Artesian Basin, Australia. We used four different machine learning algorithms (support vector
924 machine, partial least squares, gaussian process and random forest) to downscale the original
925 GRACE estimate of 0.5° to a spatial grain size of 0.1° (global) and 0.05° (regional). This was
926 based on precipitation, evapotranspiration and runoff estimates from the Famine Early Warning
927 Systems Network Land Data Assimilation System (FLDAS) and Australian Water Outlook
928 (AWO) hydrological models, respectively. The downscaled products were validated using 42
929 in-situ precipitation observations spread across the test region. We further evaluated which of
930 the downscaled products best mimicked local-scale hydrology using a range of statistical
931 metrics. Our results showed that regional hydrological models best characterized the dynamics
932 of local scale hydrology (rainfall v. downscaled product), and the gaussian process regression
933 algorithm made the best predictions for both models. The correlation coefficients for the raw
934 values varied from 0.45 to 0.49 while that of the standardized values varied from 0.46 to 0.52
935 with the random forest model providing the best fitting for the regional-based products. The
936 regional downscaling approach employed in this study may be readily integrated into local
937 water resources planning programs.

938

939