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Multivariate prediction of total water storage changes over West Africa from multi-satellite data

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Abstract West-African countries have been exposed to changes in rainfall patterns over the last decades, including a significant negative trend. This causes adverse effects on water resources of the region, for instance, reduced freshwater availability. Assessing and predicting large-scale total water storage (TWS) variations is necessary for West Africa, due to its environmental, social, and economical impacts. Hydrological models, however, may perform poorly over West Africa due to data scarcity. This study describes a new statistical, data-driven approach for predicting West African TWS changes from (past) gravity data obtained from the Gravity Recovery and Climate Experiment (GRACE), and (concurrent) rainfall data from the Tropical Rainfall Measuring Mission (TRMM) and sea surface temperature (SST) data over the Atlantic, Pacific, and Indian Oceans. The proposed method, therefore, capitalizes on the availability of remotely sensed observations for predicting monthly TWS, a quantity which is hard to observe in the field but important for measuring regional energy balance, as well as for agricultural, and water resource management. Major teleconnections within these data sets were identified using independent component analysis (ICA) and linked via low-degree autoregressive models to build a predictive framework. After a learning phase of 72 months, our approach predicted TWS from rainfall and SST data alone that fitted to the observed GRACE-TWS better than that from a global hydrological model. Our results indicated a fit of 79% and 67% for the first year prediction of the two dominant annual and inter-annual modes of TWS variations. This fit reduces to 62% and 57% for the second year of projection. The proposed approach, therefore, represents strong potential to predict the TWS over West Africa up to two years. It also has the potential to bridge the present GRACE data gaps of one month about each 162 days as well as a - hopefully - limited gap between GRACE and the GRACE follow-on mission over West Africa. The presented method could

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also be used to generate a near-real time GRACE forecast over the regions that exhibit strong teleconnections.

Keywords Predicting GRACE-TWS \cdot West Africa \cdot Autoregressive model \cdot ICA \cdot GRACE gap filling

1 1 Introduction

West African climate is highly variable, ranging from tropical to semi-arid and arid 2 over a limited 1500-km North-South gradient. The main source of precipitation 3 over a large part of West Africa (WA) is driven by the WA monsoon system and 4 tightly linked to large-scale pattern of ocean-atmosphere-land interaction (Gian-5 nini et al., 2003, 2008). Inter-decadal rainfall decrease over WA was highlighted as 6 one of the largest precipitation patterns on the planet over the last half century 7 (Ali and Lebel, 2009), leading to high risks of prolonged droughts, as in the 1970s 8 and 1980s. Moreover, global warming adds up multiple threats to the region, with 9 the duration and magnitude of droughts and floods expected to increase (Nichol-10 son, 2000, Speth et al., 2011). It is of critical importance to understand and predict 11 the impact of the WA climatic system on water resources over timescales of several 12 months, as the livelihoods of roughly 70% of the region's population depend on 13 uncertain rainfall and exposure to climate risk (Hansen et al., 2011). 14

Drought severity is classically expressed in terms of the Palmer drought index, 15 based on moisture data only (Heim 2002). However, this index does not explicitly 16 account for the state of all water storage compartments (Long et al., 2013), as 17 prolonged drought conditions may have an impact on deeper groundwater sys-18 tems even with limited anthropic pumping (Chen et al., 2010). Houborg et al. 19 (2012) showed significant interest in incorporating total water storage observa-20 tions (TWS), defined as the sum of all available water storage on and below the 21 surface of the Earth, to be used for drought monitoring. Its applicability is due to 22 the fact that TWS can represent all available forms of water resource (Scanlon et 23 al., 2012, Schuol et al., 2008), thus, might be a better representative of drought 24 compared to soil moisture or groundwater compartment alone. 25

Importance of quantifying TWS variations goes beyond its application in water 26 resource studies. In general, the internal states of storage compartments determine 27 their reaction to imposed boundary conditions. Runoff is driven by water stored in 28 soil compartment and groundwater systems. Soil moisture layers - and groundwa-29 ter to a lesser extend - also control evapotranspiration, cooling the land surface and 30 regulating local energy and water balances (Koster et al., 2004). In this sense, WA 31 has been highlighted as a 'hot spot', where the land-atmosphere coupling could 32 play an important role, through the recycling of precipitation and the modulation 33 of rainfall gradients (Douville et al., 2006). Main processes affecting rainfall and 34 water availability in WA at seasonal to decadal time scales have been extensively 35 studied within the framework of international efforts under the AMMA¹ initiative 36 (e.g. Redelsperger et al. 2006). Beside land-atmosphere coupling, WA monsoon 37 variability coincides with other overlapping shifts like those in global tempera-38 ture and natural sea surface temperature (SST) oscillations in all tropical oceans, 39

¹ African Monsoon Multidisciplinary Analysis

showing remote (Pacific) or local (Atlantic and Indian) influences (see Rodríguez-40 Fonseca et al., 2011 and references therein, Mohino et al., 2011). Diatta and Fink 41 (2014) studied the relationships between climate indices and monsoon rainfall, de-42 rived from rain gauge data, over West Africa, covering 1921 to 2009, and reported 43 positive correlations between Sahel rainfall and the Atlantic Multi-decadal Oscil-44 lation (AMO), as well as the Atlantic Meridional Mode (AMM). Their results also 45 indicated a significant impact of ENSO on inter-annual variability of precipita-46 tion over WA. Up to now, however, complex coupled ocean-atmosphere models 47 represented limited skills to accurately simulate the main SST-WA monsoon tele-48 connections, both at inter-annual and decadal scales. This is reported to be caused 49 by the simplification of different aspects of the climate system and of persistent 50 biases (e.g., Rodríguez-Fonseca et al., 2011). 51 Land surface models (LSMs) and hydrological models are commonly applied 52 to simulate the impact of climate on storage compartments (e.g., Döll et al., 2003, 53 Rodell et al., 2004, van Dijk et al., 2013). However, the quality of the models 54

strongly depends on model structure, boundary conditions (rainfall and evapo transpiration) and data availability, and also on model calibration/parametrization
 (Güntner et al., 2007). Over WA, modeling the impact of the monsoon on water
 resources is restricted by limited data for calibration/validation purposes (Boone

⁵⁹ et al., 2009, Schuol and Abbaspour, 2006), leading to large magnitude of uncer-

 $_{\rm 60}$ $\,$ tainties on the water balance and TWS.

Time-variable gravity solution of the Gravity And Climate Experiment (GRACE) 61 mission offers an opportunity to remotely measure large-scale TWS changes on re-62 gional and global scale (Tapley et al. 2004, Schmidt et al., 2008a). A few studies 63 have highlighted the critical interest of GRACE-TWS observations in WA due to 64 the sparse distribution of in situ observation network with respect to the size of 65 the region (Xie et al., 2012). Nahmani et al. (2012) showed that GRACE accu-66 rately estimates the annual variability of WS over WA, when compared to the 67 output of hydrological models and GPS observations. Grippa et al. (2011) carried 68 out a model comparison study between various GRACE products and nine land 69 surface models (LSMs) and showed substantial differences between GRACE-TWS 70 and LSMs. The differences were mainly ascribed to the weakness of the LSMs to 71 correctly simulate water in surface reservoirs and evapotranspiration during the 72 drv seasons. 73

This study presents a multivariate statistical TWS forecasting approach for 74 West Africa (WA). Our goal is to capitalize on the availability of homogeneously 75 processed, remotely sensed observations of gravity from GRACE, sea surface tem-76 perature (SST) from satellite data, as well as rainfall data from the Tropical Rain-77 fall Measuring Mission (TRMM), and predict large-scale annual and inter-annual 78 variability of West-African TWS changes up to a few years. Therefore, the term 79 'prediction' or 'forecast' in this study refers to estimation of the TWS quantity, for 80 the period that TWS has not been observed, using its indicators, which in our case 81 are SST and precipitation changes. A statistical approach, based on 'system iden-82 tification' framework (Ljung, 1987), is chosen here for our predictions (see Section 83 3) since we are interested in accurate final monthly values of TWS rather than 84 exploring the mechanism of changes in TWS compartments (e.g., soil moisture 85 and groundwater) and their interactions. A similar concept has already been used, 86 e.g., by the USA's National Oceanic and Atmospheric Administration (NOAA) 87 for predicting climatic parameters (http://www.cpc.ncep.noaa.gov/). We should 88

mention here that one could also alternatively use 'gap-filler' approaches (e.g., 89 Rietbroek et al., 2014) to estimate (or predict) surface load or TWS over a re-90 gion of interest. We will show later that the prediction approach here provides up 91 to two years TWS predictions, while retaining the spatial resolution of GRACE 92 products. Reager and Famiglietti (2013) presented an experimental predictions 93 approach that relates water storage changes to precipitation forcing and then gen-94 eralize the relation based on large-scale basin characteristics. Unlike our proposed 95 method, this approach requires extra information about basin characteristics. 96

The predictability skill of the proposed statistical approach would be optimal if 97 major physical processes over the region of study are included in the learning phase. 98 Thus, both ocean-atmosphere and land-atmosphere processes are represented as 99 predictors of West African TWS changes: (i) SST variations over the major oceanic 100 basins of the Atlantic, Pacific, and Indian Oceans (ii) TRMM rainfall observation 101 over West Africa. Although other predictors might also improve the forecasting 102 results (evapotranspiration, soil moisture changes), model quality is related to 103 parsimony and data homogeneity. Here, we only rely on SST and rainfall data since 104 they are more accurately derived from remote sensing observations compared to 105 the other possible indicators (see, e.g., Reynolds et al., 2002, Huffman and Bolvin, 106 2012, Wang and Dickinson, 2012). 107

Time-variable maps of predictors (SST and rainfall data) and predictands 108 (TWS data) include large temporal and spatial correlations. This requires ap-109 plication of a dimension reduction method before constructing the mathematical 110 relationship between predictors and predictands (e.g., Kaplan et al., 1997). This 111 considerably improves the skill of the forecasting approach (see e.g., Westra et al., 112 2008). The statistical method of independent component analysis (ICA) was ap-113 plied to extract individual modes of variability that are mutually independent and 114 successively explain the maximum amount of existing variance in the data (Fo-115 rootan and Kusche, 2012, 2013). An optimum autoregressive model with exogenous 116 variables (ARX) (Ljung, 1987) was then used to relate independent components 117 (ICs) of predictands to ICs of predictors. In the end, the model allows a thor-118 ough representation of complex processes in a highly efficient way as compared 119 to physical models. The combination of ICA/ARX modeling can be generalized 120 worldwide, with an adequate identification of likely forcing recalibration of the 121 model, with respect to the region of interest. Examples include the regions such 122 as North America and the Australian continent, which exhibit strong ocean-land-123 atmosphere interactions (Douville et al., 2006, Forootan et al., 2012). 124

From a methodological point of view, we prefer the ICA algorithm for dimen-125 sion reduction over, e.g., principal component analysis (PCA, Preisendorfer, 1988); 126 this view is rooted in the improved performance of ICA in extracting trends, an-127 nual patterns, as well as slow dynamic patterns such as the El Niño-Southern 128 Oscillation (ENSO) from climate observations (e.g., Aires et al., 2002, Ilin et al., 129 2005)). In a preliminary study, Forootan and Kusche (2012) and Forootan et al. 130 (2012) applied the ICA method to global and local GRACE-TWS time series, and 131 demonstrated its value in extracting climate related patterns. We also evaluated 132 the use of PCA in our proposed statistical TWS forecast (results are not shown 133 here), and found that ICA improves the extraction of teleconnections, e.g., ENSO 134 and the Indian Ocean Dipole (IOD) patterns, as well as the performance of the 135 prediction. A similar conclusion was reached, e.g., by Westra et al. (2007), who 136 assessed the performance of ICA and PCA for simulating hydrological time series. 137

Finally, we prefer the ARX model over the common canonical correlation analysis (CCA) approach (e.g., von Storch and Navara, 1999) for relating predictors
and predictands since ARX offers more flexibility to relate multiple parameters as
exemplified e.g., in Westra et al. (2008).

To implement our prediction approach, first, we begin by decomposing the 142 following data sets individually into statistically independent modes: (i) GRACE-143 TWS changes over West Africa, to provide the dominant independent patterns of 144 total water storage (TWS) that are subsequently identified with the predictands 145 of the ARX process; (ii) SSTs over the Atlantic, Pacific, and Indian Ocean basins, 146 in order to extract ocean-atmospheric interactions and teleconnections; and (iii) 147 TRMM data over West Africa, for extracting the main patterns of rainfall over 148 the region. Then, the modes found by analyzing (ii) and (iii) are introduced as 149 predictors of (i) within the ARX process model, while using the first 72 months 150 of (i), (ii) and (iii) for the training step (statistical simulation). The fitted ARX 151 model, along with the independent modes of SST and rainfall (i.e. the predictors 152 153 of the ARX model) after the 72'th month are then used to predict TWS after the simulation period. The prediction is evaluated using those GRACE-derived 154 TWS anomalies that are available after the simulation period. Forecasting error 155 levels are also predicted using a Monte Carlo error estimation process. We should 156 mention here that to decompose water storage and rainfall data in (i) and (iii), we 157 introduced the West Africa region as a simple box (latitude between 0° to $25^{\circ}N$ 158 and longitude between -20° to $10^{\circ}E$). The method, however, can be extended to 159 grids delineated by basin shape or basin-averaged time series. 160

This contribution is organized as follows; in Section 2, we briefly present the 161 data sets used in the study. The dimension reduction and the ARX forecasting 162 methods are introduced in Section 3, followed in Section 4 by a discussion of the 163 leading independent modes found in the total water storage (TWS), sea surface 164 temperature (SST) and rainfall data sets. In Section 5, we discuss the results of 165 ARX-TWS simulations and forecasts over West Africa. The study is concluded in 166 Section 6. The paper also contains two appendices. In Appendix A, the details of 167 GRACE-TWS estimations over West Africa are described, and in Appendix B, we 168 present the details of mathematical methods, used in this study, including ICA, 169 and the ARX model as well as their uncertainty estimations. 170

171 2 Data

¹⁷² 2.1 Total Water Storage from GRACE and WGHM

The GRACE mission consists of two low-earth orbiting satellites in the same or-173 bital plane at the current altitude of ~ 450 km and in an inclination of 89.5° . The 174 separation distance between the two satellites is measured precisely by a K-band 175 ranging system and the location of each satellite is determined by GPS receivers 176 on-board the spacecraft (Tapley et al., 2004). These data, after application of sev-177 eral corrections, are then used by a number of analysis to generate time-variable 178 (usually monthly) Level-2 gravity field products (Flechtner, 2007). In this study, 179 we used monthly GRACE products from the German Research Centre (GFZ) 180 Potsdam (Flechtner, 2007) for computing TWS fields, covering August 2002 to 181 May 2011. We did not interpolate the missing data of January 2003, 2004, May 182

2003, and December 2008 in order to avoid creating artifacts. For comparison, we 183 also used monthly GRACE-ITG2010 products from Bonn University, Germany 184 (Mayer-Gürr et al., 2010), which are available for the period between September 185 2002 and August 2009, and are provided together with full variance-covariance 186 information. The covariance matrices were used to estimate the accuracy of the 187 GRACE-TWS grids. Total water storage from GRACE are also compared with 188 TWS output from the WGHM model (Döll et al., 2003), covering the years 2003 189 to 2010. WGHM represents the major hydrological components, such as soil mois-190 ture, rainfall, snow accumulation, melting, evaporation, runoff, and the lateral 191 transport of water within river networks. For this study, we prefer WGHM over 192 using land surface models (LSM) since it also contains a groundwater simulation 193 model and, therefore, its vertically aggregated storage can be directly compared 194 to GRACE TWS. The details of data preparation are described in Appendix A. 195

196 2.2 SST

Monthly reconstructed global $1^{\circ} \times 1^{\circ}$ Reynolds sea surface temperature (SST) 197 data (Reynolds et al., 2002) were used over the period 2002 to 2012. The Reynolds 198 SST has been frequently used for climate studies, including some addressing African 199 rainfall variability in relation to SST (e.g., Mohino et al., 2011, Omondi et al., 200 2012). Similar to Omondi et al. (2012), the SST data cover three major ocean 201 basins: we include an Atlantic Ocean box $(-66^{\circ} \text{ to } 13^{\circ} \text{ E and } -20^{\circ} \text{ to } 31^{\circ} \text{ N})$, a 202 Pacific Ocean box $(159^{\circ} \text{ to } 275^{\circ} \text{ E and } -30^{\circ} \text{ to } 19^{\circ} \text{ N})$ and an Indian Ocean box 203 $(34^{\circ} \text{ to } 114^{\circ} \text{ E and } -50^{\circ} \text{ to } 1^{\circ} \text{ N})$. Sea surface temperatures in these regions are 204 then extracted and analyzed through the ICA approach (Section 4). We found that 205 a slight difference in the size of the selected boxes would not change the results of 206 ICA significantly. 207

208 2.3 TRMM

Version 7 of TRMM-3B42 products (Huffman and Bolvin, 2012) covering 2002 to 209 2012 (http://mirador.gsfc.nasa.gov/) was used. The downloaded 3-hourly rainfall 210 rates have been converted to rainfall amount and aggregated to monthly basis. 211 TRMM was previously used e.g., by Nicholson et al. (2003) to study the patterns 212 of precipitation over West Africa. Huffman and Bolvin (2012) and Fleming and 213 Awange (2013) reported a significant improvement of version 7 over version 6, 214 likely as a result of including more microwave sounding and imagery records as 215 well as implementing better processing algorithms. 216

217 3 Methodology

²¹⁸ 3.1 Identifying Dominant Independent Patterns from Available Data

²¹⁹ In order to keep the problem of identifying independent modes on a grid, in-

²²⁰ cluding the statistical relationships between them, numerically manageable, it is

²²¹ mandatory to first apply a dimension reduction method before constructing the

mathematical relationship between predictors and predictands (e.g., Kaplan et al., 1997). This improves the prediction skills of the statistical approach, since the redundant information within the data sets, both predictors and predictands, will be reduced. Dimension reduction is implemented here by applying a 2-step inde-

pendent component analysis (ICA) algorithm (Forootan and Kusche, 2012, 2013)

²²⁷ to the TWS, rainfall, and SST data sets. Forootan and Kusche (2012) formulate

two alternative ways of applying ICA, in which either temporally independent components or spatially independent components are constructed. The temporal

²³⁰ ICA method, which we simply abbreviate here as ICA, is preferred in this study ²³¹ since it provides temporally independent components that allow the development ²³² of a prediction model that is univariate in the predictand (see Section 3.2).

Let us assume that GRACE-TWS anomalies (in mm), after removing the temporal mean, are stored in the matrix $\mathbf{X}_{TWS} = \mathbf{X}_{TWS}(s, t)$, where t is the time, and s stands for spatial coordinate (grid points). Applying ICA means that \mathbf{X}_{TWS} is decomposed into spatial and temporal components as

$$\mathbf{X}_{TWS} = \mathbf{Y}_j \mathbf{A}_j^T,\tag{1}$$

where the columns of \mathbf{Y}_j contain the *j* dominant unit-less temporally independent components (ICs) of TWS, and the columns of \mathbf{A}_j represent the corresponding spatial maps. Each temporal pattern (i.e. a column of \mathbf{Y}_j) along with the corresponding spatial pattern (a column of \mathbf{A}_j) represent an independent mode of variability. Likewise, the temporally centered maps of rainfall over West Africa $\mathbf{X}_{Rainfall}$, and of SST over the major oceans \mathbf{X}_{SST} can separately be written as

$$\mathbf{X}_{SSTorRainfall} = \mathbf{U}_{j'} \mathbf{B}_{j'}^T, \tag{2}$$

where $\mathbf{U}_{j'}$ stores the j' dominant unit-less temporally independent components of SST or rainfall, and the columns of \mathbf{B}'_{j} contain the associated spatial maps. We used different indices j and j' in Eqs. (1) and (2) to emphasize that the number of retained modes from different data sets are not necessarily the same. Selecting a proper subset (j or j') is addressed in Appendix B.

In our analysis, we found the spatial patterns associated with independent 248 modes of total water storage anomalies, i.e. the columns of \mathbf{A}_{i} (Eq. (1)) to be 249 sufficiently stable. This means that, for instance, the spatial patterns (\mathbf{A}_{j}) derived 250 from 10 years of TWS data do not differ significantly from those derived from 8 251 or 12 years of data. Therefore, for building the forecasting model, we only link 252 the temporal components (ICs) of the predictor data sets (all columns of $\mathbf{U}_{j'}$ 253 derived from SSTs and TRMM-rainfall) to individual ICs of the predictand (each 254 column of \mathbf{Y}_j in Eq. (1)). Finally, we will use the \mathbf{A}_j derived from TWS in order 255 to reconstruct the forecasting maps. Details of the ICA decomposition and the 256 corresponding error estimation are addressed in Appendix B. 257

258 3.2 Prediction using an Autoregressive Model with Exogenous Variables (ARX)

²⁵⁹ An ARX process is governed by a system of linear equations, which describe the

²⁶⁰ relationship between the current and previous values of the system output and the

values of inputs. In our case, the ARX model is formulated as a multiple-input

(the independent modes or ICs of SST and rainfall all together) and single-output
(each IC of TWS) model (Ljung, 1987):

$$y(t) + \sum_{i=1}^{n_a} a_i y(t-i) = \sum_{q=1}^{m} \sum_{l=1}^{n_b} b_{q,l} u_q(t-k_q-(l-1)) + \xi(t),$$
(3)

where y represents a particular mode of TWS, i.e. y(t), t = 1, ..., n, represent 264 a column of \mathbf{Y}_{j} in Eq. (1). In Eq. (3), n_{a} is the order of the ARX model with 265 respect to the predict and, $u_q(t)$, $q = 1, \dots, m$, and $t = 1, \dots, n$, are ICs of SSTs 266 and rainfall from $\mathbf{U}_{j'}$ in Eq. (2), while m is the number of predictors. The order of 267 the ARX model with respect to the predictors is n_b , and k_q denotes the number of 268 time-steps before the q'th input (predictor) affects the output y, i.e. the dead time 269 of the system. Finally, ξ allows for a white-noise random input. The coefficients 270 of the ARX models a_i , $i = 1, \dots, n_a$, and $b_{q,l}$, $q = 1, \dots, m$, and $l = 1, \dots, n_b$, 271 have to be derived in the simulation step, using both predictand and predictors 272 (Ljung, 1987). Once the coefficients are computed, in the forecasting step only 273 the predictors (ICs of SST and rainfall) are used to estimate the values of TWS 274 after the simulation period. Details of the computations and error propagation are 275 addressed in Appendix B. 276

277 4 Dominant Independent Modes of TWS, SST, and Rainfall

When following the decomposition procedure as described in Section 3.1, we iden-278 tify two independent, statistically significant, modes in GRACE GFZ-TWS (ab-279 breviated as GFZ-TWS), four independent modes in SST changes over the Atlantic 280 Ocean, three modes over the Pacific Ocean, and four modes over the Indian Ocean. 281 For the rainfall changes, also four significant independent modes were obtained. 282 Our approach for separating significant modes from the insignificant ones is also 283 presented in Appendix B. Finally, Table 1 summarizes the variance percentage of 284 the modes discussed so far. 285

Table 1 List of the variance percentage that each of the independent mode in Section 4 represents. Independent modes of GRACE GFZ-TWS are shown in Fig. 1, a and b, those of the Atlantic, Pacific and Indian Ocean-SST are shown in Fig. 2. Fig. 3 contains the independent modes of TRMM-rainfall.

	First Independent Mode	Second Independent Mode	Third Independent Mode	Fourth Independent Mode
GRACE GFZ-TWS	62.4%	20.4%		
WGHM-TWS	60.4%	16.4%		
Atlantic Ocean-SST	46.4%	25.4%	11.7%	4.1%
Pacific Ocean-SST	55.6%	15.4%	14.6%	
Indian Ocean-SST	47.8%	15.4%	14.3%	11.1%
TRMM-rainfall	44.2%	12.3%	6.9%	6.4%

286 Dominant Independent Modes Identified in Total Water Storage Variability

²⁸⁷ The first and second independent modes the from TWS anomalies derived from

GRACE (GFZ solutions) are shown in Fig. 1,a. The first dominant independent
 mode, which explains 62.4% of variance, represents the annual water variability

²⁹⁰ over West Africa. Here a damping of the signal magnitude can be seen in the year

2005 (temporal IC1 of GRACE GFZ-TWS). From the spatial pattern of IC1, a 291 concentration of annual variability appears to be dominant over the tropic and 292 coastal regions. The second mode of GRACE-TWS contains inter-annual varia-293 tions, along with periodic components of ~ 3 and 5 years period. Nicholson (2000) 294 found a similar period in rainfall variations over West Africa. The second inde-295 pendent mode represents 20.4% of the GRACE-TWS variance, thus, the first two 296 leading modes in Fig. 1 represent more than 80% of the TWS variance over West 297 Africs. In fact, the dominanting annual and inter-annual variability of TWS are 298 found well separated, and thus can be treated separately within the ARX simula-299 tion and prediction steps. We attribute this behavior to the properties of the ICA 300 decomposition method. 301

The separate treatments of the two annual and inter-annual variability of wa-302 ter storage components seems to be reasonable since they are likely due to differ-303 ent physical influences from environment (here the indicators SST and rainfall). 304 Therefore, the mathematical relationship between TWS and its indicators must 305 be separately weighted (i.e. coefficients $a_i, i = 1, \dots, n_a$, and $b_{q,l}, q = 1, \dots, m$ of 306 IC1-GRACE and IC2-GRACE will be separately computed in Eq. 3). We would 307 like to mention here that the oscillations that exist in the extracted dominant 308 independent modes are not necessarily explained by a fundamental annual or 309 inter-annual cycle and its overtones. Therefore, for the decomposition and pre-310 diction procedures, we chose not to reduce any such pre-defined oscillations (see 311 also Schmidt et al. 2008b). 312

For comparison, we then projected WGHM-TWS and ITG2010-TWS on to the 313 spatial patterns of Fig. 1,a, using Eq. (B2) (Appendix B). The results are shown 314 by the black and gray lines in Fig. 1,a. The temporal patterns indicate that the 315 annual TWS changes from WGHM (IC1 in Fig. 1,a) are comparable to those seen 316 by GRACE, whereas at the inter-annual time scale they are different (see IC2 in 317 Fig. 1,a). To confirm this finding, we also applied ICA (Eq. (1)) to the WGHM-318 TWS data, individually, with the results shown in Fig. 1,b. The first independent 319 mode of WGHM-TWS (60.4% of variance) is comparable to that of GRACE-TWS, 320 while the second mode of WGHM-TWS (spatial and temporal pattern of IC2-321 WGHM) that accounts for 16.4% of variance is found quite different from those 322 of GRACE-TWS (both GFZ and ITG2010). This finding shows that WGHM-323 TWS and GRACE-TWS are not consistent at inter-annual time scale; compare 324 Fig. 1,a with Fig. 1,b. We hypothesize that the difference could be attributed to 325 the possible miss-modeling of surface water storage or water withdrawals over the 326 region. Further research will be needed to address the exact cause of differences, 327

³²⁸ but this is outside the scope of the current study.

329 Dominant Independent Modes of Sea Surface Temperature and Rainfall Data

Applying the ICA approach (Eq. (2)) to SST changes over the three ocean boxes 330 shows that their first two independent modes are related to the annual variability 331 of SST (IC1 and IC2 in Fig. 2,a,b, and c). Over the Atlantic, for instance, IC1 332 and IC2 are related to the annual dipole structure, which also correlate very much 333 with IC1 of GFZ-TWS. The same damping of the annual amplitude in the year 334 2005 is seen for IC2-Atlantic SST, similar as with IC1 of GFZ-TWS. Our result 335 confirms that the recent annual variability of total water storage over West Africa 336 is highly correlated with the Atlantic ocean-atmospheric interactions, reflected in 337



Fig. 1 Overview of the ICA decomposition of TWS changes over West Africa (counted as predictands). a) ICA decomposition of GRACE GFZ-TWS data (GFZ-TWS). For comparisons, WGHM-TWS and ITG2010-TWS changes are projected on the spatial patterns of IC1 and IC2, using Eq. B2 in Appendix B. The results are presented along with temporal ICs of GFZ-TWS. b) ICA decomposition of WGHM-TWS maps. The variance fraction of each independent mode is presented in Table 1. Uncertainties are shown by error-bars around temporal components. Details of uncertainty computations can be found in Appendix B.

- the SST data (see similar findings in e.g., Mohino et al., 2011). For the variance percentages that each mode represents, we refer to Table 1.
- $_{\rm 340}$ $\,$ We find that the third mode of SST changes over the Atlantic and Indian
- ³⁴¹ Ocean boxes represents semi-annual variability, while IC3-Pacific SST represents
- the ENSO pattern; we compared IC3-Pacific SST with the monthly ENSO pattern (shown by the Southern Oscillation Index (SOI)) provided by the Australian

Bureau of Meteorology (http://www.bom.gov.au/climate/enso/). A high correla-

 $_{345}$ tion of 0.84 was obtained, suggesting that the pattern is physically meaningful

³⁴⁶ (IC3 in Fig. 2,b). We also found a significant correlation of 0.68 between IC2 of ³⁴⁷ GRACE-TWS (Fig. 1,a) and SOI, revealing a relationship between total water

³⁴⁸ storage variability over West Africa and ENSO.

IC4-Atlantic SST represents a complicated pattern, which we do not attempt

to interpret here. IC4-Indian SST (Fig. 2,c) follows the Indian Ocean Dipole (IOD) pattern (see e.g., Saji et al., 1999). Comparing our results to the IOD index derived

from the Japan Agency for Marine-Earth Science and Technology (JAMSTEC,

³⁵³ http://www.jamstec.go.jp/frcgc/research/

d1/iod/HTML/Dipole%20Mode%20Index.html) represents a significant correlation of 0.73. This shows that ICA extracts teleconnection patterns from SST

356 data fairly well.

³⁵⁷ Four independent modes were extracted from TRMM-rainfall data, from which

 $_{\tt 358}$ $\,$ IC1-TRMM and IC2-TRMM relate to the annual rainfall variability with three

³⁵⁹ months phase differences (Fig. 3). In 2005, a damping of the signal magnitude can

be seen in IC2-TRMM, but it is less pronounced compared to that of IC2-Atlantic

361 SST. This might be due to the fact that IC2-TRMM represents a local impact,

³⁶² compared to the large-scale interaction that IC2-Atlantic SST represents. IC3-

TRMM and IC4-TRMM apparently represent the semi-annual rainfall variations.
 We found a lag of two months between the ICs of rainfall and those of TWS.



Fig. 2 Overview of ICA decomposition applied to the SST changes over (a) the Atlantic, (b) Pacific, and (c) Indian Oceans. The variance fraction of each independent mode is presented in Table 1. Uncertainties are shown by error-bars around temporal components. The smoothed temporal patterns in (a) and (b) are derived by applying a 12-month moving average filter.



Fig. 3 Overview of ICA decomposition applied on rainfall changes over West Africa. The variance fraction of each independent mode is presented in Table 1. Uncertainties are shown by error-bars around temporal components.

³⁶⁵ 5 Predicting Total Water Storage with an Autoregressive Model

366 Training Step

To compute the best-fitting ARX model, we have inserted the first 72 months 367 of each mode of GRACE GFZ-TWS (IC1 and IC2 in Fig. 1,a) and the first 72 368 months of all temporal modes of SST and rainfall (ICs of Figs. 2 and 3) in Eq. 369 (3). Before performing the training step of the ARX model, the data for January 370 2003, 2004, May 2003 and December 2008 were excluded from the input time series 371 (ICs of SSTs and rainfall) to synchronize them with the GFZ-TWS time series. 372 Then, we had to choose optimum n_a and n_b ; these were found experimentally by 373 varying them between one to three. The time delay k_q was searched for between 374 zero and three months. This was then followed by running the ARX simulation 375 step (Eq. (3)). We did not consider higher orders for n_a and n_b since we would 376 377 like to keep the forecasting model as simple as possible (e.g., Westra et al., 2008). For k_a , previous studies (e.g., Ahmed et al., 2011) found a delay of up to three 378 months between SST-rainfall and TWS changes. The required coefficients for each 379 ARX model Θ were computed using Eq. (B5) in Appendix B. 380

Our numerically simulated results for both IC1 and IC2 of GFZ-TWS suggest 381 that an ARX model with $n_a=1$ and $n_b=3$ provides the best fit with the residuals 382 passing the normality test. The RMS of differences between the simulated TWS 383 values from the ARX process and the ICs of GFZ-TWS (Eq. (B6) in Appendix 384 B) was used as the fit criterion. Two sets of k_q corresponding to the simulations 385 of the IC1 and IC2 of GFZ-TWS were found and are presented in Table 2. Our 386 simulation results indicate that the ARX models provide a fit of 93% and 83%387 for simulating the two dominant components of GFZ-TWS (IC1 and IC2 in Fig. 388 1,a), respectively. The simulation fit of ARX corresponding to IC2 of GFZ-TWS 389 is, however, lower than that of IC1 since its temporal pattern appears much more 390 complicated than the annual pattern in IC1. Therefore, it might not have been 391

³⁹² fully captured by the predictors (see Fig. 4).

Table 2 Time delays k_q derived from simulation of IC1-GRACE GFZ-TWS and IC2-GRACE GFZ-TWS. The values are in month and denote the number of time-steps before each predictor (ICs of SSTs and ICs of TRMM-rainfall respectively in Figs. 2 and 3) affect the output (each individual IC of GRACE GFZ-TWS in Fig. 1, a).

	IC1	IC2	IC3	IC4	IC1	IC2	IC3	IC1	IC2	IC3	IC4	IC1	IC2	IC3	IC4
	SST	SST	SST	SST	SST	SST	SST	SST	SST	SST	SST	TRMM	TRMM	TRMM	TRMM
	Atlantic	Atlantic	Atlantic	Atlantic	Pacific	Pacific	Pacific	Indian	Indian	Indian	Indian	West	West	West	West
	Ocean	Ocean	Ocean	Ocean	Ocean	Ocean	Ocean	Ocean	Ocean	Ocean	Ocean	Africa	Africa	Africa	Africa
k_q related to	1	0	2	1	0	3	1	1	0	1	0	0	3	3	1
IC1 of GFZ-TWS															
k_q related to	1	0	1	1	0	0	1	1	0	1	0	1	3	1	3
IC2 of GFZ-TWS															

To assess the sensitivity of the ARX models (Eq. (3)) with respect to each 303 input, first, for each IC of GFZ-TWS, each IC of Figs. 2 and 3 was individually 394 inserted in Eq. (3) and the ARX model evaluated. For each IC of GFZ-TWS, 395 therefore, an ensemble of 15 ARX-modeled TWS outputs was generated, and the 396 correlations of these outputs and the ICs of GFZ-TWS were then computed. From 397 the 15 ARX-generated TWS, those that represented the largest correlations with 398 their corresponding IC of GFZ-TWS were likely to have the most influence on the 399 prediction. Our results show that the ARX-outputs generated by IC1, IC2-Atlantic 400

401 SST, and IC1-rainfall had the largest influences on the ARX model of IC1 GFZ-

 $_{402}$ $\,$ TWS. The prediction of IC2 GFZ-TWS was found to be sensitive to IC3-Pacific

403 SST, IC3-Atlantic SST, and IC3-rainfall. The most sensitive indicators and the

404 correlations of the associated outputs with the ICs of GFZ-TWS are presented

 $_{405}$ in Table 3. One might use these results for model reduction of the original ARX

⁴⁰⁶ process (see e.g., Westra et al., 2008), however, such a reduction was not applied

407 in this study since (i) the fit derived from each of the 15 model run was smaller

than that of original ARX run, and (ii) the ARX models apparently possessed

 $_{409}$ $\,$ sufficient degree of freedom to be computed based on the current indicators.

Table 3 List of the most sensitive indicators derived from the ARX models for each input and the computed correlation of the output with IC1 and IC2 of GRACE GFZ-TWS. Correlations are derived at 95% level of confidence.

Rank:	1	2	3
Model run by:	IC1	IC2	IC1
	SST	SST	TRMM-rainfall
	Atlantic	Atlantic	West
	Ocean	Ocean	Africa
Correlation with	0.81	0.61	0.52
IC1 of GFZ-TWS			
Model run by:	IC3	IC3	IC3
	SST	SST	TRMM-rainfall
	Pacific	Atlantic	West
	Ocean (ENSO)	Ocean	Africa
Correlation with	0.59	0.46	0.42
IC2 of GFZ-TWS			

410 ARX Forecasting Step and Validation

Having simulated the ARX model parameters for the two dominant independent 411 modes of GFZ-TWS (Θ is known from Eq. (B5), within the training step), we used 412 the indicator time series, i.e. all ICs shown in Figs. 2 and 3 after the 72-months 413 training period alone to predict ICs of GRACE GFZ-TWS changes for the years 414 2010 and 2011. The predictions were derived from Eq. (B8), and their uncertainties 415 were evaluated using the Monte Carlo approach described in Appendix B. Training 416 and forecast results are shown in Fig. 4a,b. Our prediction approach, therefore, 417 uses only the process structure described in Section 3.2 and the determined lag 418 relation between the predictors and ICs of GFZ-TWS changes (i.e. Table 2). The 419 fit of the forecast for the first leading mode of total water storage, when compared 420 to the observed GFZ-TWS values, after one year was found 79%, while after two 421 years this reduced to 62%. As Fig. 4a also shows, after two years, the standard 422 deviation of the propagated uncertainty is quite large. This suggests that the 423 proposed approach is more or less reliable for predictions of up to two years. Fig. 424 4b shows that the fit of the forecast for the second leading independent pattern of 425 total water storage after one year was reduced to 67%. After two years, a fit of 57%426 was found. Comparing projected values of WGHM-TWS (black lines in Fig. 1a) 427 with the ICs of GFZ-TWS, during the first year of forecast, we found a fit of 78%428

Table 4 List of the computed fit values (Eq. B6) derived from comparing the ARX-TWS outputs with the IC1 and IC2 of GRACE GFZ-TWS. We also compared the projected values of WGHM-TWS in Fig. 1 with the IC1 and IC2 of GRACE GFZ-TWS. The values indicate that the ARX outputs are closer to that of GRACE GFZ-TWS.

	Simulation period	First year of the forecast	Second year of the forecast
	(12 months)		
Fit values of			
the ARX model with respect			
to IC1 of GFZ-TWS:	93%	79%	62%
Fit values of			
the ARX model with respect			
to IC2 of GFZ-TWS:	83%	67%	57%
Fit values of			
the WGHM model with respect			
to IC1 of GFZ-TWS:	91%	78%	43%
Fit values of			
the WGHM model with respect			
to IC2 of GFZ-TWS:	54%	53%	31%

for the annual and a moderate fit of 53% for the inter-annual pattern. This result
indicates that the TWS prediction from the proposed statistical method is indeed
closer to the observed GFZ-TWS changes over West Africa, when compared to
hydrological modeling. See the fit values in Table 4.

Comparing the ARX-derived TWS predictions with the ICs of GFZ-TWS, dur-433 ing the forecast period, we found no apparent deviations between TWS time series 434 (see Fig. 4a,b), thus, the reported fit values are significant. For the inter-annual 435 time-scale, however, specific care should be taken since the simulation and pre-436 diction of the ARX-TWS method is very much sensitive to the temporal patterns 437 of the input parameters. When the ICs of SSTs or rainfall are not well defined, 438 the inter-annual forecast of ARX-TWS might perform poorly or be biased. This 439 has been tested by replacing the ICs of SSTs and TRMM-rainfall with temporal 440 components derived e.g., from the principal component analysis (PCA) decompo-441 sition for running the ARX predictions (results are not shown). A bias was found 442 in the prediction of IC2 GFZ-TWS, which was most likely due to the fact that the 443 PCA-derived indicators (PCs of SST and rainfall) do not reflect the inter-annual 444 TWS changes sufficiently. 445

In order to assess the robustness of the performed forecast with respect to the 446 training period, we performed a backward simulation and forecast, i.e. the last 447 72 months of both indicators (ICs of SSTs and TRMM-rainfall) and predictands 448 (individual ICs of GFZ-TWS) were used in the simulation step to predict the first 449 two years of GFZ-TWS. The results, summarized in Fig. 5, show a fit similar to 450 the forward forecast in Table 4. Therefore, even though the training step was quite 451 short, no temporally variable bias was found in both forward and backward predic-452 tions. This confirms the robust performance of the proposed ICA-ARX approach, 453 at least, with respect to the performed tests. 454

Inserting the time series of the prediction and the spatial components of Fig. 455 1,a in Eq. (1), one may reconstruct the TWS maps for the period when the ARX 456 model and their inputs are available. In this case, our prediction values provide Y 457 and the spatial maps of Fig 1,a provide A in Eq. (1). Fig. 6 compares the original 458 GRACE GFZ-TWS values of the year 2010, after removing the temporal mean of 459 2003 to 2011 and the contribution of Lake Volta (as discussed in Section 3 and 460 Appendix A), with the values of the ARX-TWS forecast. The predictions fit quite 461 well to GFZ-TWS fields. Fig. 6,c shows the difference between GFZ-TWS and the 462 predicted ARX-TWS. The patterns of the differences are similar to the striping 463

⁴⁶⁴ noise of GRACE solutions (Kusche, 2007). Our results, therefore, support the idea

465 of using the presented statistical approach to forecast TWS changes over West

466 Africa.



Fig. 4 Results of simulations and forecasts of IC1 and IC2 of GRACE GFZ-TWS (Fig. 1,a), using the ARX models (shown by black-lines). Fig. 4a(top) represents the results for IC1 of GRACE GFZ-TWS while assuming the ICs of Figs. 2 and 3 as indicators. Fig. 4a(bottom) shows the uncertainty of the forecast on top. Fig. 4b(top) represents the same results as (a) but corresponding to IC2 of GRACE GFZ-TWS. Fig. 4b(bottom) indicates the uncertainty of the forecast on top. Fig. 72 months of TWS are used (shown in blue). TWS values after the 72th month are then used for evaluating the forecasts (shown in red). Reconstructing the forecast for the year 2010, and its comparison with the original GRACE GFZ-TWS fields are presented in Fig. 6.



Fig. 5 Backward simulations and forecasts of IC1 and IC2 of GRACE GFZ-TWS (Fig. 1,a), using the ARX models (shown by black-lines). The results are similar to those of Fig. 4, however here, the last 72 months of both indicators (ICs of SSTs and TRMM-rainfall) and predictands (individual ICs of GRACE GFZ-TWS) are used in the simulations and the first two years of IC1 and IC2 of GRACE GFZ-TWS predicted. Fig. 5a(top) represents the results for IC1 of GRACE GFZ-TWS. Fig. 5a(bottom) shows uncertainty of the forecast on top. Fig. 5b(top) represents the same results as (a) but corresponding to IC2 of GRACE GFZ-TWS. Fig. 5b(bottom) indicates the uncertainty of the forecast on top.



Fig. 6 Overview of TWS maps for the year 2010 over West Africa, without the signal of Volta, and after removing the temporal mean of 2003 to 2011. (a) TWS maps derived from GRACE (GFZ RL04 data), (b) TWS maps derived from the statistical forecast (the ARX models and ICA results), and (c) the differences between (a) and (b).

467 6 Conclusions and Outlooks

This study suggests and investigates a new statistical multivariate seasonal fore-468 casting approach for total water storage (TWS), which uses sea surface tempera-469 ture and rainfall data alone to estimate TWS changes over West Africa. The pro-470 posed ICA/ARX approach does not directly simulate the complex physical process 471 of ocean-land-atmosphere, but instead, it statistically learns the relationships be-472 tween main known physical processes of the region (such as teleconnections and 473 the soil-precipitation feedback) and uses it to predict TWS (the parameter of in-474 terest). The successful implementation of the proposed ICA/ARX approach relies 475 on the proper selection of TWS indicators and avoiding over-parametrization of 476 the model, data homogeneity and a learning phase that contains a thorough range 477 of processes and impacts. Therefore, the dependence of the statistical model on the 478 climate characteristics of the calibration period is often referred as a lack of model 479 robustness. To investigate this issue, we performed a numerical validation, which 480 showed that the seasonal forecast of TWS is close to TWS that is actually mea-481 sured by GRACE, see Table 4. Both forward and backward predictions indicate 482 that the proposed approach provides relatively stable large-scale seasonal TWS 483 forecast over West Africa. We also carried out an extensive uncertainty analysis 484 and were able to show that the predictability skills of the model is stable. However, 485 due to the estimated uncertainties, the results might not be significant after about 486 one year of forecast. We would like to mention here that the proposed method 487 is only able to provide predictions of total water storage, therefore, hydrological 488 modeling would still be required to partition TWS into different compartments. 489 Since the prediction method relies on the relationships between SST and rainfall as 490 indicators of TWS, we expect that the ICA/ARX method, with its current param-491 eterization, is most appropriate to be used over those regions that exhibit strong 492 interactions between ocean-atmosphere and land water storage changes, which is 493 the case over West Africa. 494

Since the proposed method is trained on GRACE products, it provides rela-495 tively coarse resolution TWS maps. The approach also assumes that the spatial 496 pattern of TWS changes remains stationary within the two years of the forecast. 497 Before application, one should therefore analyze whether this assumption is ful-498 filled for different time frames. This can be achieved by applying the ICA technique 499 to TWS time series of different length, and evaluating whether the dominant spa-500 tial patterns appear indeed invariant. Another issue is that the training of the 501 ARX model was performed based on six years of the data. Since SST and rain-502 fall are available for a longer period (e.g., for TRMM, since 1998), one could use 503 TWS outputs of models for the time before 2002.8 and extend the training period. 504 Addressing the impact of such extension in terms of the quality of the ARX coeffi-505 cients and the consistency of the model-derived TWS with GRACE-TWS requires 506 further research. 507

Our numerical results lead us to the hope that the presented statistical method could be helpful for filling the current gaps of the GRACE products (once every 162 days, with one or two months of data is missing) and a possible gap period between GRACE and its successor mission GRACE-FO at least for certain regions such as West Africa. Another application of the presented approach could be the generation of near-real time GRACE forecasts. Product latency time of GRACE fields is currently two to three months, while using the suggested approach, one could be able to forecast GRACE total water storage maps immediately as soon
as rainfall and sea surface temperature data become available. Such near-real time
predictions could be used for various drought/flood monitoring applications. Generating total water storage predictions, close to GRACE products, would also
be possible by calibrating and/or assimilating GRACE products in hydrological
models. Models improved in this way could then be used to simulate total water

⁵²¹ storage. Examples of such implementations can be found in studies, e.g., Zaitchik

et al. (2008), Werth et al. (2009b), Houborg et al. (2012), and Xie et al. (2012). The computational load of such approaches is however much more heavier than

with the proposed statistical ICA/ARX approach.

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739 Appendix A (Computational Details of Total Water Storage Fields)

In order to prepare the data sets for analysis, the following processing steps were
 applied.

The GRACE Level-2 data that are used here, are derived in terms of fully normalized spherical harmonic (SH) coefficients of the geopotential fields (Flechtner, 2007). Firstly, the fields were augmented by the degree-1 term from Rietbroek et al. (2009) in order to include the variation of the Earth's center of mass with respect to a crust-fixed reference system.

GRACE SHs at higher degrees are affected by correlated noise and are, there-747 fore, smoothed by applying the DDK2 decorrelation filter (Kusche et al., 2009). 748 Werth et al. (2009a) found that the DDK2-filtered GRACE solutions are gen-749 erally in good agreement with the output of global hydrological models. How-750 ever, GRACE solutions are also contaminated by errors due to incomplete 751 reduction of short-term mass variations by de-aliasing models (Forootan et al., 752 2013, 2014). We found that the impact of atmospheric de-aliasing errors on the 753 GRACE-derived TWS over West Africa is negligible (see atmospheric errors 754 over the Niger Basin in Forootan et al., 2014). 755

- GRACE DDK2 filtered solutions up to degree and order 120 were then used
 to generate the global TWS values according to the approach of Wahr et al.
 (1998).

- Similar to the GRACE products above, the DDK2 filter was applied to the
 gridded WGHM-TWS data set in order to preserve exactly the same spectral
 content as with the filtered GRACE products.

- ⁷⁶² After filtering, all data sets were converted to $0.5^{\circ} \times 0.5^{\circ}$ grids similar to the ⁷⁶³ WGHM-TWS outputs.
- ⁷⁶⁴ From each data set, a rectangular region that includes West Africa (latitude ⁷⁶⁵ between 0° to $25^{\circ}N$ and longitude between -20° to $10^{\circ}E$) was selected.

Lake Volta (see Fig. A1) is one of the largest man-made reservoirs in the world, 766 created by the Akosombo Dam, which holds back the water for generating hydro-767 electric power (for details see Speth et al., 2011). Satellite altimetry observations 768 indicate a sharp increase of water level since mid 2007, where much of the excess 769 water resulted from heavy rainfall within the catchment (Crétaux et al., 2011). 770 This introduces an artificial TWS anomaly located over the lake, which is removed 771 to avoid its misinterpretation as a part of subsurface TWS changes. The equivalent 772 water height (EWH) change of Volta was computed by assuming a grid mask 773 representing a unit change in EWH of 1 mm over the entire lake surface and zero 774 elsewhere. The grid mask has been converted into a set of spherical harmonic 775 coefficients up to degree 120 and subsequently filtered using the same DDK2 filter 776 used for filtering the original GRACE-TWS data. Then, each field was scaled 777 using the lake height time-series (in mm) derived from the results of Crétaux et al. 778 (2011). The averaged storage changes derived from GRACE-TWS (from GFZ) and 779 altimetry are shown in Fig. A1. Both altimetry and GRACE GFZ-TWS indicate 780 an increase of water storage within the lake. The amplitude of the signal derived 781 from GRACE GFZ-TWS is larger than that of the altimetry likely since GRACE-782 TWS also reflects the groundwater signal of the surrounding area of the lake. For 783 the lake area, we estimate a TWS increase of $2.95 \pm 1.32 \ km^3 yr^{-1}$, during 2003 784

to 2010. The time series of Lake Volta water storage changes were then removed

⁷⁸⁶ from GRACE-TWS fields (including both GFZ and ITG2010).



Figure A1: Overview of water storage changes of Volta Lake. The graph on top shows the location of the lake, while that of the bottom-left compares the averaged contribution of Volta lake level changes (derived from altimetry in black) with the averaged TWS variations derived from GRACE (GFZ-TWS products, in red). The bottom-right graph shows the GRACE GFZ-TWS signal after removing the water storage signal of Lake Volta.

In order to compare the signal strength over the region, the signal root-mean-787 square value (RMS) and the linear trend of the three mentioned TWS data sets 788 (GFZ, ITG2010 and WGHM) are computed for the period January 2003 to August 789 2009, in which the three data sets were available (see Fig. A2). From the RMS, one 790 concludes that all the three data sets show a strong variability over the tropical 791 and the Gulf of Guinea coastal regions. The computed linear trends, however, 792 are not consistent. Particularly, GRACE-derived TWS changes show a mass gain 793 over Volta Lake, which we remove from the GRACE-TWS fields before performing 794 decomposition. Removing such artificial anomaly is necessary, since otherwise the 795 amplitude of TWS forecast over the lake will be overestimated. 796



Figure A2: Comparing the signal variability (RMS) and linear trends of TWS data used in this study after smoothing using the Kusche et al. [2009]'s DDK2 filter. (A) TWS data of GRACE GFZ RL04, (B) TWS data of GRACE ITG2010, and (C) TWS of WGHM.

797 Appendix B (Details of ICA and ARX Methods)

 $_{798}$ $\,$ This appendix provides details of computations regarding to the methodology

⁷⁹⁹ described in Section 3.

800 The ICA Computations

ICA decomposition is performed here by applying a 2-step algorithm (Forootan and Kusche, 2012) on the available data sets, where step 1 consists of data decorrelation using principal component analysis (PCA). In step 2, the *j*-dominant components of PCA are rotated to be as independent from each other as possible. Storing the available data in a $n \times p$ data matrix **X**, after removing their temporal mean, where *n* is the number of months and *p* is the number of grid points, ICA decomposes **X** as

$$\mathbf{X} \simeq \mathbf{X}_j = \bar{\mathbf{P}}_j \mathbf{R}_j \mathbf{\Lambda}_j \mathbf{R}_j^T \bar{\mathbf{E}}_j^T.$$
(B1)

In Eq. (B1), $\bar{\mathbf{P}}_{i} \mathbf{\Lambda}_{i} \bar{\mathbf{E}}_{i}^{T}$ is derived from the PCA decomposition of **X** in step 1. 808 Therefore, Λ_j is an $j \times j$ diagonal matrix that stores the singular values arranged 809 with respect to the magnitude, \mathbf{E}_{i} $(j \times p)$ contains the corresponding unit-length 810 spatial eigenvectors, $\bar{\mathbf{P}}_{i}$ $(n \times j)$ contains the associated normalized temporal com-811 ponents, and j < n is the number of retained dominant modes (Preisendorfer, 812 1988). The orthogonal rotation matrix $\hat{\mathbf{R}}_{i}$ $(j \times j)$ is defined in step 2, so that it 813 rotates PCs and make them as statistically independent as possible. The method 814 equals to temporal ICA (Forootan and Kusche, 2012), which is simply called ICA 815 in the paper. Considering Eqs. (1) and (2), \mathbf{Y} and \mathbf{U} are equivalent to $\mathbf{\bar{P}R}$, while 816 A and B are equivalent to $\Lambda \overline{E} R$. An optimum R was found by digonalization 817 of the fourth-order cross cumulants of the dominant temporal components $\bar{\mathbf{P}}$ (see 818 details in Forootan and Kusche, 2012). 819

For properly selecting the subspace dimension j or j', we used a Monte Carlo 820 approach which simulates data from a random distribution $N(0, \Sigma)$, with Σ con-821 taining the column variance of \mathbf{X} . The null hypothesis is that \mathbf{X} is drawn from 822 such a distribution (see also Preisendorfer, 1988, pages 199 to 205). To apply 823 the rule, 100 time series realizations of $N(0, \Sigma)$ are generated, their eigenvalues 824 computed and placed in decreasing order. The 95th and 5th percentile of the cu-825 mulative distribution are then plotted (red lines in Fig. B1). Eigenvalues from the 826 actual data sets that are above the derived confidence boundaries are unlikely to 827 result from a data set consisting of only noise. To estimate the uncertainties of 828 the eigenvalues, we randomly selected a subsample of \mathbf{X} and applied PCA, then 829 selected another subsample and repeated this operation 200 times. This approach 830 follows the 'bootstrapping' method as presented, e.g., in Efron (1979) and yields 831 uncertainty estimates (see error-bars in Fig. B1). The repeat number of 200 is cho-832 sen experimentally to be sure that the distribution of the estimated eigenvalues is 833 independent from the selections of the subsamples. 834

To illustrate what we describe above, Fig. B1 shows the eigenvalue spectrum of the centered time series of GRACE GFZ-derived TWS, SST and rainfall computed using PCA. The significance levels are shown by red lines and the error-bars show the uncertainties of eigenvalues. The eigenvalues above the red lines are statistically significant. The significant eigenvalues along with their orthogonal components are rotated towards independence using Eq. (B1) and interpreted in Section 4.

Based on the uncertainties of the PCA results (Fig. B1), in order to estimate the uncertainty of the ICs (Eq. (B1)), we generated 100 realizations of **X**, reconstructed by $\bar{\mathbf{P}}_j$, Λ_j , and $\bar{\mathbf{E}}_j$ along with 100 realizations of their errors. Then, applying Eq.



Figure B1: Eigenvalue results derived from implementing the PCA method on (a) time series of GRACE GFZ-TWS maps, (b) maps of SST over the Atlantic, (c) maps of SST over the Pacific, (d) maps of SST over the Indian Ocean basins, and (e) West-African rainfall maps from TRMM. Uncertainties are shown by error-bars around each eigenvalues. The red lines correspond to the significant test, described in Appendix B. The variance fractions of the dominant eigenvalues are represented in each graph.

(B1) to the realizations allows the estimation of uncertainties (see, e.g., error-bars in Figs. 1, 2, and 3).

The projection of the data **X** onto the i'th spatial pattern of the ICA $\hat{\mathbf{p}}_i = \mathbf{X}\hat{\mathbf{e}}_i$, provides its corresponding temporal evolution

$$\hat{\mathbf{p}}_i(t) = \sum_{s=1}^p x(t,s) \,\hat{\mathbf{e}}_i(s),\tag{B2}$$

where t is time $(1, \dots, n)$ and s is the number of grid points $(1, \dots, p)$.

849 The ARX Computations

⁸⁵⁰ Considering Eq. (3) as the ARX model, the ARX-forecast requires two steps: ⁸⁵¹ (i) The coefficients (a_1, \dots, a_{n_a}) and $(b_{q,1}, b_{q,2}, \dots, b_{q,n_b}), q = 1, \dots, m$ are es-⁸⁵² timated, e.g., using a least squares approach. This step is usually referred to as ⁸⁵³ 'simulation' or 'training step' in literature (see, e.g., Ljung, 1987). Step (i) is per-⁸⁵⁴ formed under the assumption that the output and inputs up to the time $t = t_n - 1$ ⁸⁵⁵ are known. Furthermore, the outputs and exogenous values on the right hand side of Eq. (3) are not stochastic. To avoid negative indices, one might consider the observations $\mathbf{y}(t) = [y(t), y(t-1), \cdots, y(c)]^T$, where $c = max(n_a, n_b) + max(k_q) + 1$. Eq. (3) is expanded as

$$\mathbf{y} = \begin{bmatrix} -y(t-1) \cdots & -y(t-n_a) & u_q(t-k_q) \cdots & u_q(t-k_q-n_b+1) \\ -y(t-2) \cdots & -y(t-n_a-1) & u_q(t-k_q-1) \cdots & u_q(t-k_q-n_b) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -y(c-1) \cdots & -y(c-n_a) & u_q(c-k_q) & \cdots & u_q(c-k_q-n_b+1) \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_{n_a} \\ b_{q,1} \\ \vdots \\ b_{q,n_b} \end{bmatrix} + \mathbf{\Xi}(t), \quad (B3)$$

where $q = 1, \dots, m$ and $\Xi(t) = [\xi(t), \xi(t-1), \dots, \xi(c)]^T$. Eq. (B3) can be rewritten compactly as

$$\mathbf{y}(t) = \mathbf{\Phi}(t)\mathbf{\Theta} + \mathbf{\Xi}(t). \tag{B4}$$

⁸⁶¹ The least squares estimation of the unknown coefficients is derived from

$$\hat{\boldsymbol{\Theta}} = \left(\boldsymbol{\Phi}(t)^T \boldsymbol{\Phi}(t)\right)^{-1} \boldsymbol{\Phi}(t)^T \mathbf{y}(t).$$
(B5)

The quality of the fit (η) can be assessed by computing the signal-to-noise ratio as

$$\eta = 1 - \frac{\mathbf{y}(t)^T \mathbf{\Phi}(t) \hat{\mathbf{\Theta}}}{\mathbf{y}(t)^T \mathbf{y}(t)}.$$
(B6)

The residual of the ARX model $(\hat{\boldsymbol{\Xi}}(t) = [\hat{\boldsymbol{\xi}}(t), \hat{\boldsymbol{\xi}}(t-1), \cdots, \hat{\boldsymbol{\xi}}(c)]^T)$ can be estimated as

$$\hat{\boldsymbol{\Xi}}(t) = \boldsymbol{y}(t) - \boldsymbol{\Phi}(t) \,\hat{\boldsymbol{\Theta}}.\tag{B7}$$

In step (ii), based on $\hat{\Theta} = \begin{bmatrix} \hat{a}_1 & \dots & \hat{a}_{n_a} & \hat{b}_{q,1} & \hat{b}_{q,2} & \dots & \hat{b}_{q,n_b} \end{bmatrix}^T$, when the inputs $u_q(t)$ are known, one can forecast the output $\hat{y}(t_n)$ at time t_n using

$$\hat{y}(t_n) = -\sum_{i=1}^{n_a} \hat{a}_i y(t_n - i) + \sum_{q=1}^m \sum_{l=1}^{n_b} \hat{b}_{q,l} u_q(t_n - k_q - (l-1)).$$
(B8)

To estimate the uncertainty of the ARX simulation, using Monte Carlo sampling, we numerically generate several realizations of the ICs (described before). By inserting them into Eq. (3) and fitting ARX models, we are able to perform an error assessment of the fitted model up to the time t_n . For error estimation of the forecast (the ARX value at the time $t_n + 1$ and later), however, one should compute an accumulated error, since there is no observed value for the output y at time $t_n + 1$ and later.