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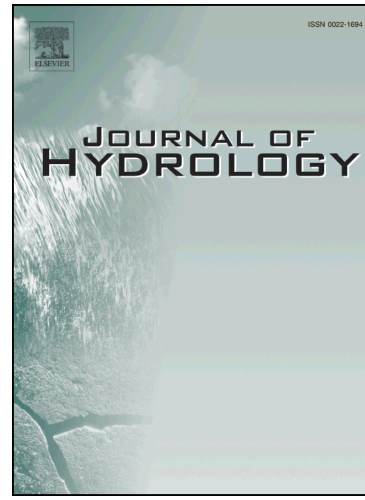

Estimation of GRACE Water Storage Components by Temporal Decomposition

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Abstract

The Gravity Recovery and Climate Experiment (GRACE) has been in operation since 2002. Water storage estimates are calculated from gravity anomalies detected by the operating satellites and although not the true resolution, can be presented as 100 km x 100 km data cells if appropriate scaling functions are applied. Estimating total water storage has shown to be highly useful in detecting hydrological variations and trends. However, a limitation is that GRACE does not provide information as to where the water is stored in the vertical profile. We aim to partition the total water storage from GRACE into water storage components. We use a wavelet filter to decompose the GRACE data and partition it into various water storage components including soil water and groundwater. Storage components from the Australian Water Resources Assessment (AWRA) model are used as a reference for the decompositions of total storage data across Australia. Results show a clear improvement in using decomposed GRACE data instead of raw GRACE data when compared against total water storage outputs from the AWRA model. The method has potential to improve GRACE applications including a means to test various large scale hydrological models as well as helping to analyse floods, droughts and other hydrological conditions.

Key words

GRACE, wavelet analysis, soil moisture, groundwater storage, decomposition, stepwise regression

1. Introduction

The Gravity Recovery and Climate Experiment (GRACE) has been in operation since 2002. Although it was originally planned to be a 5 year mission (Tapley et al., 2004), it still runs today (2017). Obtained monthly observations of the Earth's gravity field are spatially correlated with water on the Earth's surface and in subsurface layers, allowing estimations of total water storage (TWS) expressed as equivalent water thickness to be derived (Reager et al., 2015). TWS is the sum of all water stored in a GRACE cell regardless of how or where it is stored, i.e. surface water, soil water, groundwater and vegetation-bound water are all together in one TWS value (Rodell & Famiglietti, 2001). In recent years, GRACE TWS data has been used widely in many studies across many fields of science. GRACE is now a valued tool for scientists in a number of earth science fields (Wouters et al., 2014). It has been well validated against in situ, modelled and remotely sensed data (Seoane, et al., 2013; Awange, et al., 2011; Döll et al. 2014; Long et al. 2015; Long et al. 2017). A summary of relevant literature regarding the estimation of individual or multiple water storage for varying applications using GRACE TWS is presented in Table 1.

While GRACE has proven to be a very useful tool for hydrology and other sciences, it has limitations (Awange et al., 2009) and the ability to only estimate vertically integrated terrestrial water storage is a particular one. Partitioning of these TWS values into individual or smaller storage components would enhance the potential of GRACE applications. Although, Yeh et al. (2006) used GRACE to measure only a single component, groundwater, there are no documented method to comprehensively 'partition' GRACE data into multiple desired water storage components using a technique such as wavelet decomposition.

Measuring the variability in water storage across Australia has long proven to be a challenge (Cruetzfeldt et al., 2012). With limited water resources across the country (Chiew et al., 2011), it is important to understand where water is stored so that the best strategic water management actions can be applied. Hydrological models play an important role in water storage estimation across Australia. Physically based models are generally most relevant at the basin scale (Ragettli & Pellicciotti, 2012), where an appropriate amount of in situ data are more easily collected. There is a need for reliable estimates of various water storage components that can be easily applied and which have little or no dependence on field data collection.

In this paper, we aim to develop a partitioning method for estimating different vertical water storage components of GRACE TWS data. These components include, but are not limited to (1) shallow soil moisture and (2) deep soil moisture and unconfined aquifer water storage. We propose to use wavelet analysis to decompose GRACE TWS data, based on the assumption that soil moisture and groundwater at different depths have different temporal characteristics. The idea is that a wavelet analysis can decompose a time series into various temporal frequencies ranging from short (monthly) to long (seasonal – biannual), relative to the original time series (Wang & Ding, 2003). Decomposed GRACE data are statistically compared to the Australian Water Resources (AWRA) Model with the hypothesis that different combinations of decomposed temporal components correlate well to different storage components in the AWRA model and can be used to formulate storage estimations.

Table 1: A summary of relevant literature in the field of estimating individual or multiple water storage components for varying applications using GRACE TWS.

Study	***Relevant Aims***	***Study duration and size***	***Method/Approach***	***Major outcomes related to this study***
(Eicker et al., 2016)	Isolating and removing the contribution of El Nino on GRACE data	2003 – 2012 Global	Contributions of El Nino to GRACE TWS are discovered using an independent component analysis, then removed from GRACE TWS	El Nino explains roughly 24% of non seasonal variations and more accurate TWS estimations are given after its removal
(Famiglietti et al., 2011)	Estimate the groundwater component of GRACE TWS to better monitor depletion	2003-2010, California, 154,000 km^2	Measured snow and surface water values and modelled soil moisture values are subtracted from GRACE TWS to isolate groundwater estimations.	Groundwater depletion close to previous model based estimates
(Feng et al., 2013)	Estimate the groundwater component of GRACE TWS to better monitor depletion	2003-2010, Northern China, 370,000 km^2	Simulated soil moisture changes are removed from GRACE TWS to obtain groundwater estimates.	Groundwater depletion in deep aquifers is similar to what was previously estimated.
(Forootan et al., 2012)	Separate GRACE TWS signals from those of the surrounding ocean	2002-2012, Australia	An independent component analysis is applied to GRACE TWS data	Spatially independent patterns are extracted from GRACE TWS data using the independent component analysis
(Frappart et al., 2011)	Separate atmospheric, oceanic and terrestrial water storage from noise	2002-2009, Global	An independent component analysis based filter is used to partition GRACE into subcomponents	The independent component analysis is a very effective method for separating TWS from noise

(Houborg et al., 2012)	Improve drought indicators by decomposing TWS into different vertical components.	2002-2009, North America.	GRACE observations are assimilated into a climate land surface model.	The model shows a modest but statistically significant improvement in groundwater and soil moisture estimations.
(Leblanc et al., 2009)	Observe a multi-year drought and its impact on multiple water stores.	2000-2008, Murray Darling Basin ~ 1 million km^2	GRACE TWS is used alongside hydrological observations and land surface models to help infer drought severity.	GRACE TWS trends correlate highly to a basin scale simulated water depletion in groundwater, soil moisture and surface water. GRACE helps to provide integrated drought observations.
(Long et al., 2016)	Improve estimations of groundwater depletion by coupling GACE with other techniques	2003-2013, Northwest India Aquifer ~438,000 km^2	GRACE is used in conjunction with constrained forward modelling and soil moisture storage from GLDAS-1 Noah is subtracted.	The method produces results more consistent with in ground measurements, and previous estimates of groundwater depletion in the area may have been overestimated in the area.
(Reager et al., 2015)	State disaggregation of the vertically-integrated TWS.	2002-2014, Northern Plains of the USA	GRACE observations are assimilated into a climate land surface model.	Groundwater and root zone soil moisture estimates of the model assimilated with GRACE generally agree with field observations.
(Rodell et al., 2006)	Estimate the groundwater component of GRACE TWS	2002-2005, Mississippi, 900,000 km^2	Estimations of soil moisture and snow are subtracted from GRACE TWS to estimate groundwater storage changes.	Groundwater estimates from GRACE compare favourably to 58 monitored wells around the study area.
(Schrama et al., 2007)	To identify signals and noise in GRACE potential coefficient sets	2003-2006Global	An empirical orthogonal function approximation method to extract the most significant eigenvectors from the data.	Errors in GRACE data are significantly larger than simulated background model errors derived from ocean tide and atmospheric pressure models.

(Swenson et al., 2008)	Estimate the groundwater component of GRACE TWS	2002-2006, Oklahoma over 280,000 km^2	Soil moisture is estimated over the area using a network of soil moisture probes. This is subtracted from GRACE TWS to give regional groundwater estimates	Results align well with measurements from local groundwater wells showing relative inter-annual variability.
(Syed et al., 2008)	GRACE TWS is partitioned into snow, soil and canopy water storage	2002-2004, Global	GRACE is assimilated with NOAH land surface model	GRACE based storage estimates agree with modelled estimates.
(Yeh et al., 2006)	Estimate the groundwater component of GRACE TWS to better monitor storage.	2002-2005, Illinois, 200,000 km^2	Soil moisture is subtracted from GRACE TWS to estimate groundwater. Uniquely (at the time) only in situ measurements soil moisture measurements are used, not models.	Groundwater estimations perform relatively well against well based observations $r^2 = .63$.
This Study	Decompose GRACE TWS into shallow soil water and deep soil water + groundwater	2002-2013, Australia, 650,000 km^2	Wavelet decomposition is used to provide new storage estimations based on stepwise regression and a reference model as opposed to subtracting TWS components	For each of the desired components (shallow soil water and deep soil water + groundwater) the method provides estimates which perform significantly better than raw GRCE TWS values alone.

2. Data

2.1 GRACE Data

We use GRACE total water storage (TWS) data from The University of Texas Centre for Space Research (CSR), which can be freely downloaded from the GRACE Tellus website (http://grace.csr.nasa.gov/data/get-data/). Data has already been post-processed (Swenson & Wahr, 2006). Signal attenuation and leakage errors are mitigated by applying the scaling functions provided by Landerer & Swenson (2012). We used the monthly time series of TWS from March 2003 to December 2014. The data are presented spatially in 100 km by 100 km grid cells. We selected which cells should be included based on a shape file of Australia. If at least two thirds of the cell was part of the continent they were included, this eliminated some cells which covered only a small coastal part.

There are a few occurrences of a month of data missing in the CSR data set. These months were filled in by averaging the values for each cell from the months either side of the missing data. Because of the monthly temporal resolution this was deemed appropriate and maintained the average seasonal cycle well (Long et al., 2015).

2.2 AWRA Model Data

The AWRA model is a comprehensive, Australia-wide model of various water storage components (Vaze et al., 2013). Van Dijk et al. (2011) tested the performance of the AWRA model compared to GRACE and found it to be reasonably well matched in most areas, with the exception of a smaller seasonal amplitude in the AWRA model which also underestimated some storage changes after unusual high rainfall. Forootan et al. (2012) also observed a high correlation between GRACE TWS anomalies and the AWRA model. The AWRA model is calibrated using both remote sensing data and field observations. The model's documentation states that every effort has been made to prioritise the use of field measurements where possible. The AWRA model is deemed appropriate as a reference for the different sources of water storage within GRACE TWS.

The output of the AWRA at daily resolution and a cell size of .05 degree, roughly 5 by 5 km, was supplied by CSIRO (Van Dijk , 2010). Outputs include hydrological storages and fluxes in groundwater, soil, vegetation and the atmosphere. We focus on the soil and groundwater storage components and select to analyse four storage components; surface soil water **(S0)** (0-0.1 m), shallow soil water **(Ss)** (0.1-1 m), deep soil water **(Sd)** (1m-unconfined aquifer) and the unconfined aquifer **(Sg)**. To make the data comparable to the GRACE data, those cells that lay within the area of a single GRACE cell were averaged to match the GRACE resolution. Monthly averages of these cells were taken to match the temporal resolution. This was again based on an Australia shape file and only those cells where at least two thirds of the cell was part of the continent were included. The temporal extent of AWRA data matched the GRACE data, 2003 – 2014.

2.3 In situ soil moisture data

In situ soil moisture data from Aldinga, South Australia was used to demonstrate the method. The soil moisture measurements were taken with capacitance probes at seven depths: 0.1 m, 0.3 m, 0.5 m (shallow), 0.7 m and 1.1 m, 1.5 m and 2.5 m (deep). Roughly 31,000 data points at 15-minute intervals from November 2011 to September 2012 were condensed to 310 daily values. Soil moisture data was split into two layers, 'shallow' and 'deep' according to their response to rainfall events. The top three layers showed soil moisture peaks in response to rainfall, and the bottom four did not. Given as a moisture percentage, the values were converted to mm based on the depths of the measurement points.

3. Methodology

The steps involved in the study are outlined in figure 1, and explained in greater detail thereafter.

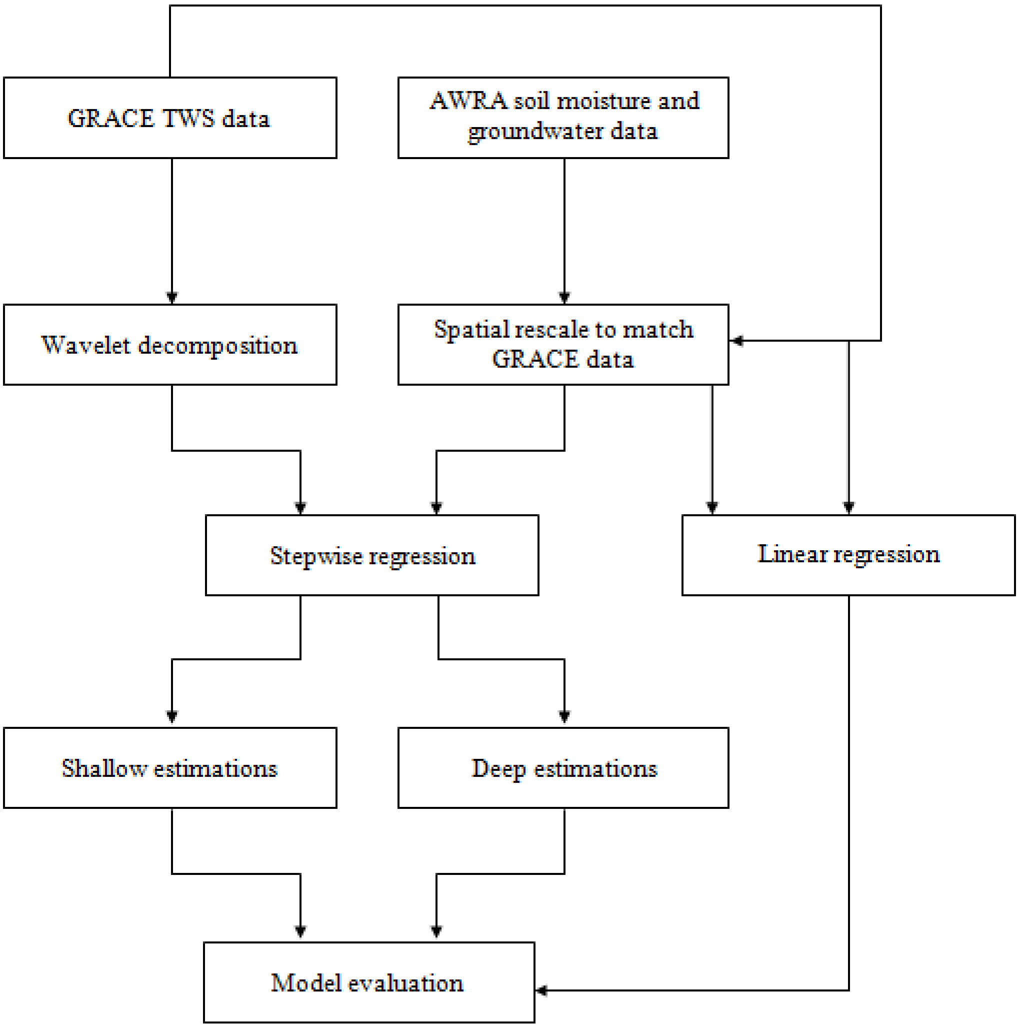

Figure 1: An outline of the steps involved in this study.

3.1 Wavelet Decomposition

The first step was to decompose the GRACE TWS data into different temporal components using a discrete wavelet transform. The method expresses decompositions as a multitude of smaller 'waves' at different frequencies (He et al., 2013). The Meyer wavelet is applied here to decompose GRACE TWS into components at different temporal scales and is suitable for this temporal data (He & Guan, 2013). This is relatively easy to achieve by means of a simple MATLAB code using the 'wavdec' function. Data are decomposed into four 'approximation' and 'detail' components, each having a different temporal scale. Approximation series maintain trends in the data while detail series neglect trends (Nalley et al., 2012). The resulting time series are labelled A1, A2, A3, A4 and D1, D2, D3 D4 for approximations and details respectively, with the time scale increasing with the decomposition number e.g. A1/D1 (2-month scale), A2/D2 (4-month scale), A3/D3 (8-month scale) and A4/D4 (16-month scale). Four levels can be reasonably extracted given the data length and monthly frequency of the data. Further decomposition would result in roughly 3- and 6-year time scales which are too coarse for a time series of only 11 years of raw data. The wavelet decomposition results in eight new time series, which can be compared to the AWRA model components, as well as with the original GRACE data.

3.2 Stepwise regression

We initially used a stepwise regression for every cell with one of the four AWRA model components at a time as the dependant variable and the eight decomposed GRACE outputs as predictor variables. In various early tests we found that the results from using **S0** and **Ss** were similar. The same was true for **Sd** and **Sg**. To simplify the experiment we decided to sum **S0** and **Ss**, and **Sd** and **Sg** together, creating 2 new storage components from the AWRA model, $\mathbf{S_{shallow}}$ **(S0 + Ss)** and $\mathbf{S_{deep}}$ **(Sd+Sg).**

3.3 Demonstration of the method using in situ soil moisture data

The method was tested using both in situ soil moisture measurements from a single site. The length of the time series was not long enough to support the common way of splitting the data into a training and validation sets by using the first half of the data for training and second half for validation. Hence, an alternating approach was adopted instead in which even days were used in the initial stepwise regressions as the training set. Based on the 'p-values' of each regression, variables which should stay in the final estimations were selected and others are excluded. The results of the stepwise regressions were then tested using odd days/months as a validation set. This produced new estimations of soil moisture for the various depths based on the decomposed sum of the soil moisture data.

3.4 Demonstration of the method on a large scale

To justify the idea of using the decomposed GRACE instead of raw GRACE data, $S_{shallow}$ and S_{deep} were summed **(S_{all})** and statistically analysed against both raw and decomposed GRACE data with a similar stepwise regression method as above with even months used in the training set and odd months used for validation. New TWS estimates were made based on the results of the stepwise regression. R^2 values and root mean squared error (RMSE) were determined for the raw data and decomposed TWS estimation compared to (S_{all}) from the AWRA model. This was a proof of concept test, it does not benefit the overall aim as it does not estimate water storage in different layers, but serves to show whether there is an improvement in the estimation by using decomposed GRACE data instead of raw GRACE data.

3.5 Estimating TWS components on a large scale

Estimations of $S_{shallow}$ and S_{deep} for every cell across Australia were made using the stepwise regression method above. The GRACE TWS decompositions were used as predictor variables and the $S_{shallow}$ and S_{deep} components of the AWRA model were used as dependant variables relatively. Again, even months used in the training set and odd months used for validation. Estimations of the water storage in the shallow and deep components were made calculated equation 1 with the selected predictor variables.

$$Y = \beta_0 + \beta_i X_i \ldots + \varepsilon \quad (1)$$

Where Y is the estimates storage value, β_0 is the intercept, β_i is the slope of variable i, X_i is the independent variable i and ε is the error.

We primarily use a Nash Sutcliffe Efficiency (NSE) for every cell to test the newly estimated water storage components against the AWRA modelled data for the same (odd) days/months. A NSE above 0 suggests that the regression performs better than the mean of the original dataset, with a value of 1 being the most outstanding fit (Legates & McCabe Jr., 1999). We also calculate RMSE for the new estimations for comparison with the AWRA dataset. The NSE is calculated as shown in equation 2,

$$E = 1.0 - \frac{\sum_{i=1}^{N}(O_i - P_i)^2}{\sum_{i=1}^{N}(O_i - \bar{O}_i)^2} \quad (2)$$

where E is the NSE, O_i is the observed value at time i, P_i is the estimated value at time i and $\bar{O}$ is the mean of the observed values.

4. Results

4.1 Concept Demonstration

Figure 2 shows an example of a 4-level wavelet decomposition. 144 months of raw GRACE data are decomposed resulting in 4 different detail (Ds) and 4 different approximation (As) coefficients.

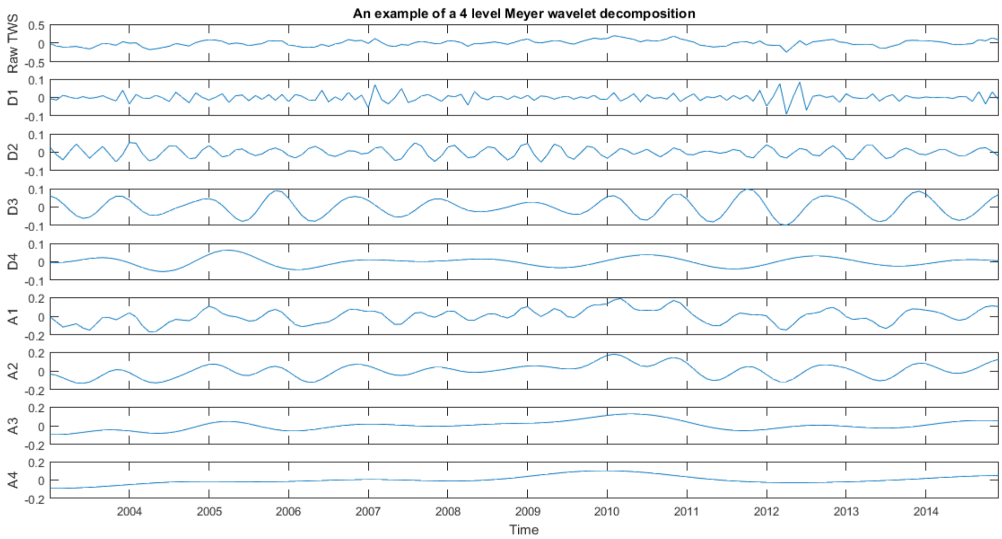

Figure 2: An example of a wavelet decomposition from the western-most cell in Australia (S 23.5°, E113.5°). Notice the visible trends in the approximations, which are normalised in the details.

A test of the method using soil moisture data from Aldinga Scrub demonstrates the improvement to estimations that can made using the method (Figure 3). High frequency variables are exclusively included in the top layer estimation (D1, A1) but D4 and D6 are also included. Only low frequency data are included in the bottom layer estimate (D4, A6, D7). The inclusion of variables D4 and A6 in both ‘shallow’ and ‘deep’ shows that the method allows for overlap of trends and frequencies between them.

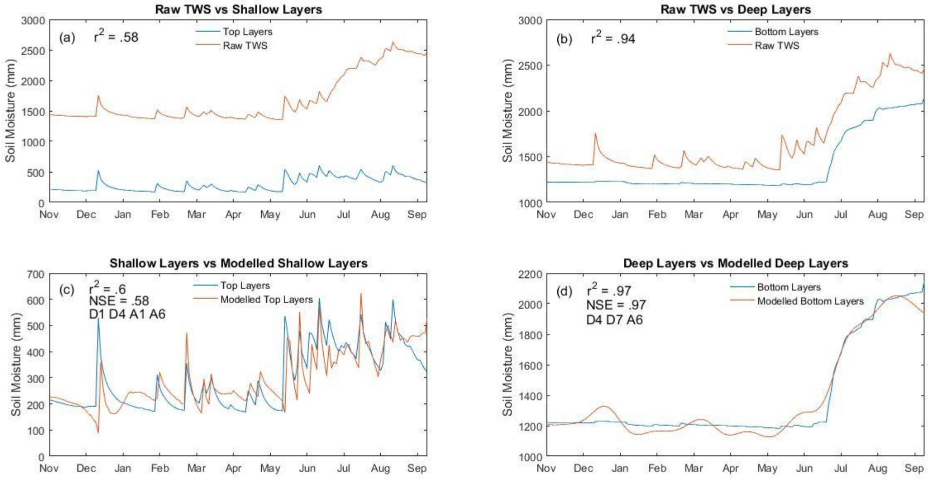

Figure 3: Results using the wavelet decomposition and stepwise regression method for estimates of soil moisture at different depths. Plots a and b show the soil TWS vs the shallow and deep layers. Plots c and d show the estimations of the shallow and deep soil layers. The r^2 value is increased using the estimation method and both display high Nash Sutcliffe Efficiencies.

The result from the first large scale proof of concept test, which compared both raw and decomposed GRACE data with the AWRA model shows a clear improvement in correlation and RMSE when the selected decomposed data are used (Figure. 4). The R^2 values increased across the entire study area, while a few regions sit well above the 1:1 line. The decomposed GRACE data also shows an overall decrease in the RMSE with a clear trend of values moving below the 1:1 line. The student-t tests confirm that the results were statistically highly significant with a *t*-statistics and *p* values of respectively 10.86 and $< 10^{-5}$ for the R^2 test and 4.422 and $<10^{-4}$ for the RMSE test.

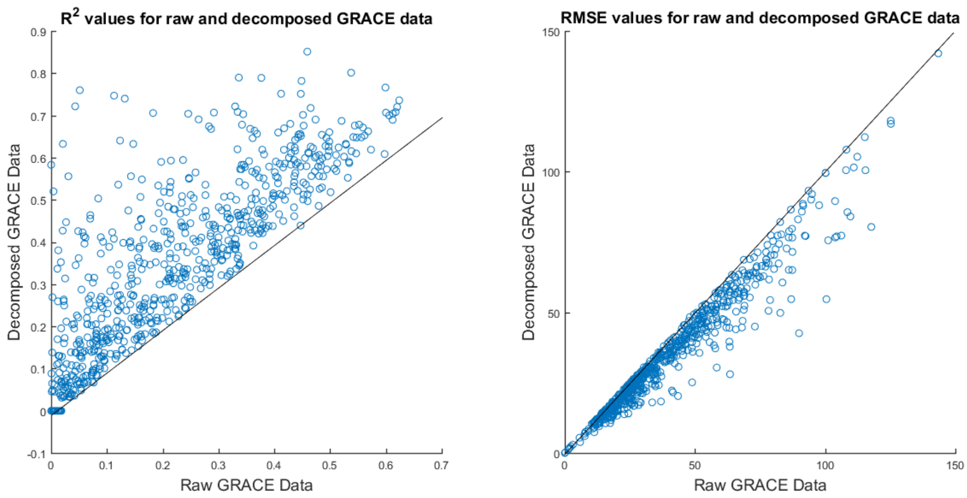

Figure 4: (a) results from the proof of concept test. R^2 values for estimations of all water storage components using raw GRACE data vs R^2 values for estimations of all water storage components using decomposed GRACE data. (b) RMSE for estimations of all water storage components using raw GRACE data vs RMSE for estimations of all water storage components using decomposed GRACE data. The decomposed GRACE data shows a clear improvement in R^2 values and a decrease of the RMSE.

As the AWRA data used in the test is the sum of the four water storage components, there is no intention that it should provide any new estimations, after all we are essentially comparing two different versions of TWS. The results are simply a demonstration of how the decomposed GRACE data can serve as an improved version of raw GRACE data.

For the second large scale proof of concept test, new total water storage estimations were produced for $S_{shallow} + S_{deep}$ using the odd months of data. These based on stepwise regressions using the even months for training data. The results for the estimations of $S_{shallow} + S_{deep}$ show that in general there is an improvement in using decomposed GRACE data for the estimation of water storage compared to raw GRACE data (Figure 5). Again, at this stage the storage components are not split and the result simply further demonstrates the concept and ability of the method.

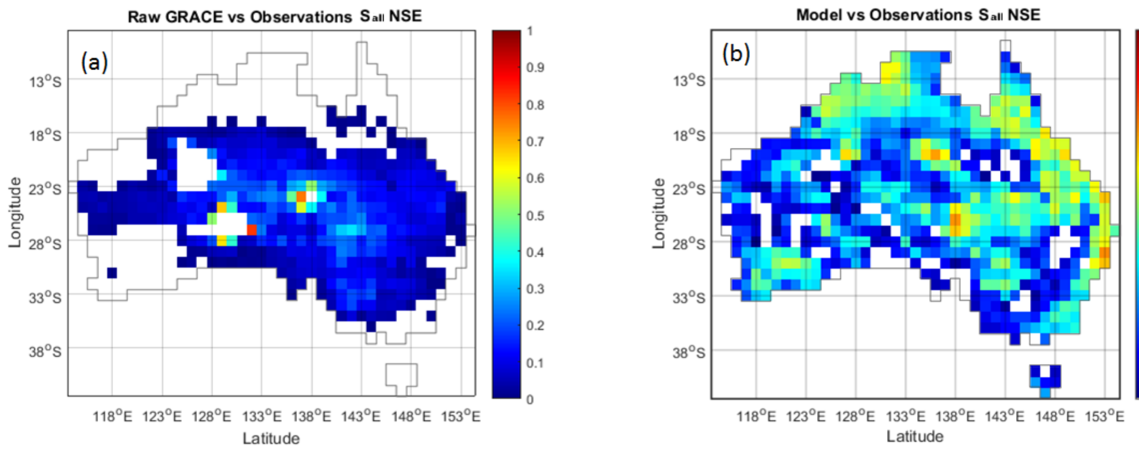

Figure 5: (a) NSE values for raw GRACE data compared to the sum of all four AWRA model water storage components. The results are generally poor with few values above 0 and many negative NSEs (depicted by white areas within the boundary). (b) NSE values for the sum of all decomposed GRACE values compared to the sum of all four AWRA model values. The results are well improved with higher values across the continent and fewer negative NSEs.

4.2 Applying the method on a large scale

An important part of running a stepwise regression is finding out which of the decomposed GRACE time series' are used in the estimations. The decompositions that are included also provide information about the behaviour of water spatially. For $S_{shallow}$, the included predictor variables for each cell were quite varied (Figure 6). There are a small number of cells which include decompositions or variables in the estimations but that do not pertain to any pattern or clustering. The variable with most cells in the estimations is D4. These cells show a strong spatial coherence. As $S_{shallow}$ represents the soil moisture in the top metre of soil, it is highly dynamic due to infiltration and evapotranspiration; the residence time for the soil water is minimal. Hence, it is unexpected that we do not see in more cells with D1 included, which pertains to a smaller temporal frequency. A possible explanation is a root water uptake occurring at a similar rate to that of infiltration.

Because detailed coefficients remove any trends it is reasonable that we see so many cells that include D4, which roughly represents a bi-annual frequency reflecting yearly wet and dry periods. The second most significant variable is D3 which roughly corresponds to a seasonal frequency, with a large cluster of included cells across the northern part of the continent. Though not quite in the tropics, Northern Australia does receive more rainfall than other parts of the country. It is reasonable to assume that D3 is included in this part of the continent simply as an extension of D4, i.e. more rainfall results in a greater range of frequencies. With more rain in this area it does not follow such a strict seasonal or annual cycle as other parts of the continent.

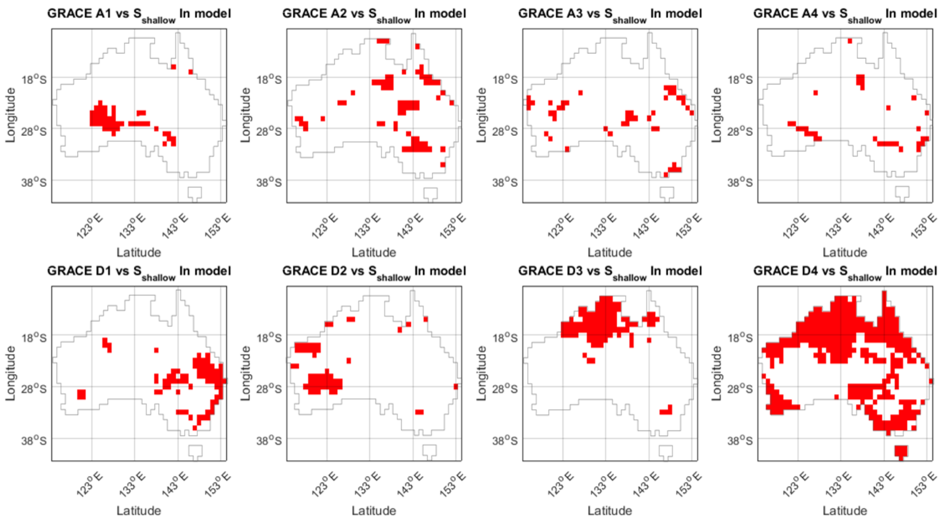

Figure 6: For each GRACE decomposition the areas that are included in the stepwise regressions for the estimation of $S_{shallow}$ are highlighted in red. Although spatially varying the most important variables are D4, followed by D3 and D1.

The comparison between the estimated $S_{shallow}$ storage component and the shallow storage of the AWRA model shows a wide range of NSE's across the continent, from average, slightly above 0, to very good, above 0.9 (Figure 7). Areas with high NSE's are observed in the northern most part of the continent, the south west corner of Western Australia and most of the coastal fringe. NSE's are lowest in central Western Australia. They are also average or close to 0 throughout central Australia and along the coast of the Great Australian Bight in the southern part of the continent.

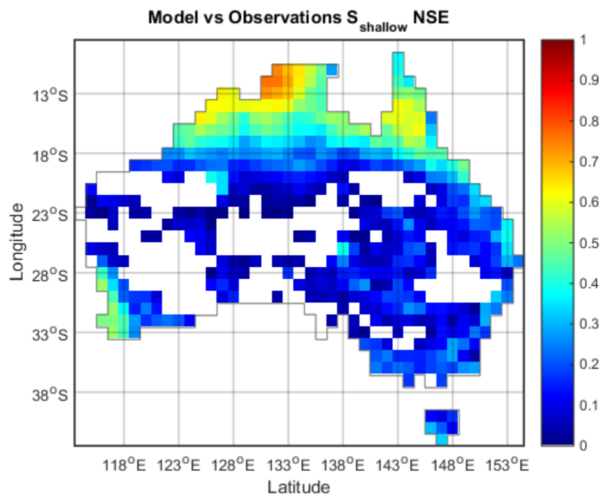

Figure 7: Nash Sutcliffe efficiencies for $S_{shallow}$ estimation compared to the AWRA model. Results show strong spatial structure with the highest NSE's located in the north, south west and scattered throughout the east of the continent. NSEs equal to or less than zero are depicted by white areas within the boundary.

The predictor variables which are included in the regression for S_{deep} are not as varied as in $S_{shallow}$, mainly A4 and D1 are selected (Figure 8). The dominance of A4 is exactly what is expected for deep soil and groundwater. A4 has roughly an annual resolution, but unlike D4 it maintains any trends in the data and hence represents slow moving nature of deep soil water and groundwater. There are however some spatially coherent areas in which A4 is not included in the estimations. These areas include northeast Australia as well as southern and northern parts of Western Australia. In most areas with A4 in the estimations, D1 is also selected. D1 is included in areas throughout Queensland and Western Australia that did not include A4. D1 represents a trendless time series with roughly a monthly temporal scale. This could suggest that deep percolation in the AWRA model corresponds to the D1 scale.

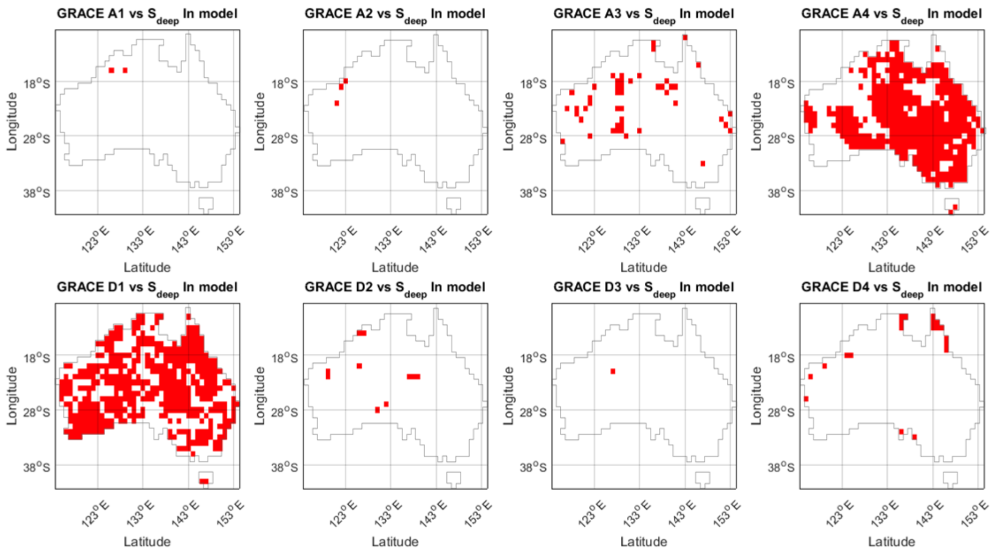

Figure 8: Areas for each variable that are selected for the estimations of S_{deep} by stepwise regressions are highlighted in red. For S_{deep} there is a very strong, continent-wide inclusion of A4 and D1 as well as an interesting inclusion of D4 almost exclusively around the coast.

S_{deep} also shows a range of spatially varying NSE's ranging from average to very good (Figure 9). There is a very large cluster of high NSE's on the eastern half of the continent. These span from Queensland, through New South Wales and Victoria and into South Australia. Another very well performing area is through southwest Western Australia, as well as parts of central Western Australia and the Northern Territory. Areas of poorer performance include the northern-most area of the continent, parts of Western Australia and parts of Central Australia. Even where the NSE's are lower, there are a minimal number of areas with a negative NSE, meaning the estimation's performance is still good overall.

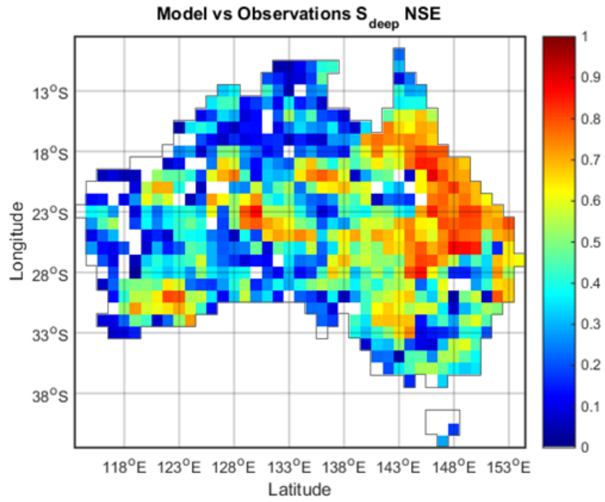

Figure 9: Nash Sutcliffe Efficiencies for each for the comparison of the S_{deep} estimations versus the AWRA model. Results are best through the Great Artesian Basin, South-Western Australia and central parts of the continent. NSEs equal to or less than zero are depicted by white areas within the boundary.

For both $S_{shallow}$ and S_{deep}, water storage estimations performed well in many areas across the continent. The relatively clear spatial clustering of good and average performing areas increases the confidence in the estimations and demonstrate the opportunity to explain the spatial patterns. Areas of weak performance tell us that the decomposed GRACE data was unable to estimate the various water storage components corresponding to the simulated storage components of the AWRA model.

5. Discussion

Though the aim of this paper is not to evaluate the AWRA model, we must consider that a possible reason for areas with lower NSE's could be a result of inaccuracies in the AWRA model. For example, for $S_{shallow}$ the areas of high NSE in part have a relationship to well populated areas. It is expected that the AWRA model is less well constrained in rural/unpopulated areas where field measurements are scarce, leading to an apparent lower performance of the decomposed GRACE estimations. A similar situation exists for S_{deep}. Some of the best performance of the estimations occurs in the Great Artesian Basin and

Murray Darling Basin, areas that have been heavily monitored in recent times and where data are abundant.

The same method could be applied using other models as a reference whether it be for Australia or anywhere else globally due to the coverage of GRACE. The range of results would vary depending on the layers included in the reference model, e.g. it could include vegetation or more specific vertical depths layers. It has the potential to be used for testing/calibrating large scale models with similar vertical layering, which can be altered depending on the reference model used. This would be particularly useful for areas where a model is largely reliant on interpolation of data or models which rely on strong assumptions in their initial conditions or parameterisation.

The separation of GRACE water storage components extends its use in many applications such as a more detailed spatiotemporal estimation of the quantitative status of the water resources. Groundwater generally makes up that largest part of the water storage and has the largest changes (Leblanc et al., 2009). As such quantifying this storage component is often of paramount importance. Famiglietti et al. (2011), Swenson et al. (2008), Rodell et al. (2006) and Feng et al. (2013) all estimate the groundwater component of different areas using GRACE TWS. Each subtracts various unwanted simulated (and/or measured) storage components from TWS to derive groundwater storage estimations. Yeh et al. (2006) do not use simulated data in their study, but solely rely on in situ measurements in an attempt to be less dependent on assumptions or poor interpolations produced by models. As such GRACE alone may provide a more reliable indicator of water status such as drought than looking at storage components individually (Long et al. 2013).

While previous results are promising, the level of success is determined by the quality of the model used and/or the data measured. This is a problem partially fixed by decomposing GRACE TWS and using significant variables to create estimations. The need for interpolation is limited due to the reference models' spatial equivalent to GRACE data. Of course a similar problem potentially exists as the estimations can only be as good as the quality of the reference model, which may have been constructed based on large interpolations, assumptions and estimates. On the other hand the method can be expanded to as many different components as exist in a suitable reference model, making it highly versatile. Another potential limitation of the method is when the assumption that shallow and deep moisture stores change at different temporal frequencies is not met. For example, results are likely to be poor where shallow soil moisture and groundwater have a similar phase of change.

GRACE has been previously used to study ecosystem performance which is largely contributed by shallow water availability, as opposed to deep soil moisture and groundwater (Yang, et al., 2014). The ability to identify the component of GRACE TWS that would contribute to shallow water availability potentially gives significant improvement in the applicability and confidence of using GRACE as a tool for this purpose.

For the same reason, partitioning GRACE into different vertical layers could also improve the application of GRACE in studying floods. Infiltration limitation and saturation excess are the two main drivers of flooding (Reager, et al., 2015). Knowing how close to saturation the near-surface soil layers are can create a better understanding of how vulnerable an area is to flooding (Fitzjohn, et al., 1998). This has not previously been an option using data at large scales as GRACE.

Studying droughts is another application of GRACE (Thomas, et al., 2014)**,** which could benefit from the separation of storage components. Similar to the application for flood studies, knowing which water stores are depleted allows for a better understanding of the severity and type of drought. Droughts are defined in many different ways throughout the world (Dracup et al., 1980), so a large range of options to quantify them is desirable. Furthermore, different regions have different water stores. In a groundwater dependent region, knowing that depleted shallow soil moisture and surface water are the main contributors to a lowered TWS while deep groundwater remains relatively stable is highly valuable information that could not be achieved using raw GRACE TWS alone. For example, Multi-year droughts in the Colorado River Basin were caused predominately by depletion of surface water and soil moisture in parts of the basin (Scanlon et al. 2015). Droughts (and other aspects of hydrology) extend to multiple disciplines such as agriculture, geography and meteorology (Dai, 2011). This means that the method we present has potential to benefit a much broader range of disciplines than GRACE is typically used for.

6. Conclusion

We aimed to develop a new method for estimating various water storage components across Australia using decomposed GRACE data, with the AWRA model as a reference. The stepwise regression was successful in determining which variables should be used in the estimation of different storage components across the continent. A simple analysis of the decomposed GRACE data compared to raw GRACE data showed that decomposing the data improved its correlation to the AWRA, increasing R^2 values and decreasing the RMSE. The estimations for $S_{shallow}$ and S_{deep} showed varying results with regard to the new estimations' performance, ranging from average to very good. The spatial clustering of the results allowed interpretation and understanding of poor estimation performance, which could be linked to areas where the AWRA model is likely less reliable. This opens the opportunity for this methodology to be applied as a tool in various hydrological applications including testing of other hydrological models.

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Table 1: A summary of relevant literature in the field of estimating individual or multiple water storage components for varying applications using GRACE TWS.

Figure 1: An outline of the steps involved in this study.

Figure 2: An example of a wavelet decomposition from the western-most cell in Australia (S 23.5°, E113.5°). Notice the visible trends in the approximations, which are normalised in the details.

Figure 3: (a) results from the proof of concept test. R^2 values for estimations of All water storage components using raw GRACE data vs R^2 values for estimations of all water storage components using decomposed GRACE data. (b) RMSE for estimations of All water storage components using raw GRACE data vs RMSE for estimations of all water storage components using decomposed GRACE data. The decomposed GRACE data shows a clear improvement in R^2 values and a decrease of the RMSE.

Figure 4: (a) NSE values for raw GRACE data compared to the sum of all four AWRA model water storage components. The results are generally poor with few values above 0 and many negative NSEs (depicted by white cells within the boundary). (b) NSE values for the sum of all decomposed GRACE values compared to the sum of all four AWRA model values. The results are well improved with higher values across the continent and fewer negative NSEs.

Figure 5: Results using the wavelet decomposition and stepwise regression method for estimates of soil moisture at different depths. Plots a and b show the soil TWS vs the shallow and deep layers. Plots c and d show the estimations of the shallow and deep soil layers. The r^2 value is increased using the estimation method and both display high Nash Sutcliffe Efficiencies.

Figure 6: For each GRACE decomposition the cells (in red) are highlighted that are included in the stepwise regressions for the estimation of $S_{shallow}$. Although spatially varying the most important variables are D4, followed by D3 and D1.

Figure 7: Nash Sutcliffe efficiencies for each cell for the $S_{shallow}$ estimation compared to the AWRA model. Results show strong spatial structure with the highest NSE’s located in the north, south west and scattered throughout the east of the continent. NSEs equal to or less than zero are depicted by white cells within the boundary.

Figure 8: Cells for each variable that are selected for the estimations of S_{deep} by stepwise regressions are highlighted in red. For S_{deep} there is a very strong, continent-wide inclusion of A4 and D1 as well as an interesting inclusion of D4 almost exclusively around the coast.

Figure 9: Nash Sutcliffe Efficiencies for each cell for the comparison of the S_{deep} estimations versus the AWRA model. Results are best through the Great Artesian Basin, South-Western Australia and central parts of the continent. NSEs equal to or less than zero are depicted by white cells within the boundary.

- Wavelet decomposition is use to split total water storage into different components
- Decomposed data performs better than raw when compared to a reference model
- This study expands the potential use of GRACE for articulating drought impacts on the root zone and groundwater.