Large-scale response of ecosystem production to GRACE derived dynamic water storage

Robert Andrew

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Faculty of Science and Engineering,

Flinders University,

South Australia

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Summary

Terrestrial ecosystems play a large role in the global carbon cycle as one of the two natural carbon sinks on Earth, along with oceans. In comparison to the ocean sink, the terrestrial carbon sink is much more variable, and often driven by temporal variations in hydro-meteorological conditions. Thus, it is important to monitor, understand, and model the hydrologically driven vegetation dynamics as a premise for improving our understanding of the global carbon cycle. Terrestrial primary production from vegetation is driven by water and in some parts of the globe is almost entirely dependent on water availability. Thus there is a clear link between terrestrial water availability and vegetation dynamics.

Our ability to estimate water storage over the globe has increased over recent decades, with the launch of remote sensing tools such as the Gravity Recovery and Climate Experiment (GRACE). GRACE has proven to be an extremely useful satellite mission for hydrological studies. The body of this research encompasses developments in our understanding of the way vegetation responds to water availability, and expands the use of GRACE data for hydrological estimations. GRACE data is analysed in an innovative way such that more information can be extracted from it than ever before. The aim of this PhD is to improve our understanding of relationships between terrestrial water and vegetation on a continental and global scale. This is in conjunction with the aim of extending the potential application of GRACE by using it in innovative and previously unused ways. Specifically, this work investigates: (1) the use of wavelet decomposition of GRACE data to comprehensively 'split' GRACE total water storage (TWS) into shallow and deep subsurface components; (2) the use of wavelet decomposition of GRACE data in conjunction with the Normalised Difference Vegetation Index (NDVI) to examine the temporal variability and moisture dependence of vegetation cover across Australia;

and (3) the use of GRACE TWS amplitude to represent dynamic water storage and to examine how it is a key driver of biomass production in terrestrial water limited ecosystems globally.

A potential limitation of GRACE is that the TWS storage it estimates have no vertical segregation. In the first component of this research, a new method was developed to create estimations of deep and shallow subsurface water storage from GRACE TWS estimations. To achieve this, a wavelet decomposition is used to 'split' GRACE into components of different temporal frequencies, hypothesising that various vertical water storage components have different temporal frequencies. For example, deep groundwater has a low frequency, slow moving signal, while the storage of soil moisture near the surface is more dynamic. The Australian Water Resources Assessment (AWRA) model is used as a reference for the decompositions of total water storage across Australia. A stepwise regression compares the wavelet decomposed components of GRACE TWS to the AWRA model. Results show a clear improvement in using decomposed GRACE data instead of raw GRACE data when compared against the outputs from the AWRA model.

GRACE TWS has recently been used to investigate moisture dependence of vegetation cover. However, part of GRACE TWS is beyond the reach of the root zone and thus irrelevant to vegetation function. In the second part of this research, this issue is addressed by using shallower water storage signals to examine temporal variability of NDVI. Wavelet decomposed components of GRACE TWS anomalies are analysed against NDVI anomalies in a stepwise regression. The results show that combinations of different frequencies of decomposed GRACE TWS data explain NDVI temporal variations better than raw GRACE TWS alone. Different types of vegetation show distinct differences in how they respond to the changes in water storage which are generally consistent with our physical understanding.

GRACE TWS of each cell is referenced to (offset by) a prescribed mean of itself, leading to difficulties to compare TWS across cells or use TWS to investigate spatial variability of vegetation cover. In the third part of this research, the hypothesis is posed that terrestrial ecosystem production is driven by effective water fluxes going through the system at a pace relevant to vegetation functioning. Hence, the relationship between the annual amplitude of GRACE TWS and gross primary productivity is examined. The GRACE amplitude represents the dynamic water storage in a year. The results show that the dynamic water storage is a significant driver of biomass production. Strong correlations between gross primary production and annual amplitudes of total water storage exist in water limited ecosystems globally. The use of total water storage amplitude provides a novel approach linking the dependence of vegetation production to water that is available and actually used by ecosystems, and extend the applicability of GRACE data in explaining large-scale spatial variability of vegetation cover.

This PhD research presents advances in our understanding of largescale water-vegetation relations which are of global significance. The innovative analysis of GRACE data as developed and, tested and applied in this research helps to shape further scientific developments in the application of such data.

Declaration

I certify that this thesis does not incorporate without acknowledgment any material previously submitted for a degree or diploma in any university; and that to the best of my knowledge and belief it does not contain any material previously published or written by another person except where due reference is made in the text

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Robert Andrew

Co-authorship

This PhD thesis was produced as a series of journal publications in leading international scientific journals. At the time of submission the progression of each chapter is as follows;

- Chapter 2: Published in *Journal of Hydrology*

  Andrew, R. A., Guan, H., and Batelaan, O., 2017. Estimation of GRACE water storage components by temporal decomposition. Journal of Hydrology, *552*, 341-350.

- Chapter 3: Accepted for publication in *Hydrology and Earth System Sciences*

- Chapter 4: Prepared for submission to a relevant journal

I am the first author on all journal publications and was responsible for leading and conducting the majority of research contained in them, including the final write up and journal submissions of the research.

The papers in this thesis have benefitted from ongoing advice and input of my supervisors, co-authors and the peer review process. I acknowledge their valuable advice and important contributions.

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1. Introduction

1.1 Background

Vegetation plays an important role in in the carbon cycle as the largest natural carbon sink and regulator of greenhouse gasses (Pan et al., 2011). Furthermore, vegetation houses many ecological, social and economic services in providing food, medicine, timber, hydrological cycle regulation, soil regeneration, recreational opportunities, and aesthetic benefits (Bonan., 2008). Vegetation and water are intimately coupled and changes in one often bring about changes in the other (Newman et al., 2006). The terrestrial water cycle plays a vital role in the climate, biology and biogeochemistry of the planet (Vörösmarty & Sahagian, 2000). Because of this, there is a need to understand dynamic interactions between the terrestrial biosphere and the water cycle (Gerten et al., 2003). Global anthropogenic induced changes such as climate change, land use change, including vegetation clearance have altered and continue to alter the amount of terrestrial vegetation. Water is a key limiting factor in the productivity in terrestrial ecosystems, and drives vegetation production (Heimann & Reichstein, 2008). Increases in drought and heat stress associated with climate change risk increased tree mortality, lowering global carbon sequestration (Allen et al., 2010). This was seen during Australia's millennium drought from 2001 – 2009, when remotely sensed vegetation cover severely decreased throughout the continent as water resources diminished (Van Dijk et al., 2013). Our ability to further understand how different water sources affect vegetation dynamics, and how vegetation responds to various changes in water availability is of paramount importance.

Over recent decades, the implementation of satellite remote sensing tools has brought new insights and information to environmental monitoring at a continental and global scale.

The Gravity Recovery and Climate Experiment (GRACE) provides monthly gridded total water storage estimates globally. The GRACE mission consists of two satellites, 'Tom' and 'Jerry' who orbit the planet and measure the gravitational pull from the Earth, which varies according to changes in mass on the planet (Tapley et al., 2004). As large mass changes are assumed to have a hydrological cause, GRACE data is produced as terrestrial water storage (TWS) for cells sized roughly 100 km by 100 km (1 degree) globally. Terrestrial and aqua versions are available. Originally planned as a 5 year mission (Tapley et al., 2004), the success and proven usefulness it has brought to the scientific community means that it is still in operation today. One most notable application is the ability to monitor groundwater depletion over large spatial areas, e.g. large parts of India are shown to suffer from overexploitation (Rodell et al., 2009). As useful as GRACE is, it comes with limitations (Awange et al., 2009). GRACE TWS estimates are generally considered acceptably accurate once the appropriate smoothing functions are applied (Whar et al., 2006). However, its ability to only estimate total water storage with no vertical differentiation is a potential limitation for some applications. One solution to this limitation is presented in this thesis.

Aside from GRACE other remote sensing tools such as the Moderate Resolution Imaging Spectroradiometer (MODIS) have provided an array of global data products. These advances in data estimation allow for valuable comparisons to be made, particularly for processes that are partially/primarily water driven, such as vegetation production.

The contents of this thesis encompasses developments in our understanding of the way vegetation responds the water availability, and expanding the use of GRACE for hydrological analysis. In a time of global climate change, the research presented is highly beneficial to the studies of vegetation dynamics, ecohydrology and climate sciences.

1.2 Research Aims

The overall aim of this PhD is to improve our understanding of relationships between terrestrial water and vegetation on a continental and global scale. The methodological aim is therefore to extend the potential use of GRACE by using it in innovative and previously unused ways in studying relationships between terrestrial water and vegetation. These aims are achieved through three individual studies with different but related focusses. In each case, GRACE is used with other datasets to make scientific advancements in large scale ecohydrology. Specific aims for each study are:

i. To partition GRACE TWS data into different vertical components, expanding its potential and creating new, useful water storage estimations. This is achieved by decomposing the GRACE TWS time series data into different temporal components which are analysed against different vertically defined storage parameters from a hydrological model.

ii. To reveal the moisture dependence of vegetation cover at different temporal frequencies. This is achieved by decomposing the GRACE TWS time series data into different temporal components which are analysed against NDVI in areas of different land use.

iii. To expose dynamic water storage as a driver of biomass production in water limited ecosystems globally. This is achieved by using the annual GRACE TWS amplitude to represent dynamic water storage and Gross Primary Production

(GPP) to represent biomass production. The two are temporally and spatially analysed for a correlation.

The studies that address these aims and knowledge gaps are presented respectively in chapters 2, 3 and 4 of this thesis.

1.3 Contribution of this Phd

This PhD research contributes towards an advanced understanding of hydrological processes at a continental and global scale, particularly relating to interactions between terrestrial moisture storage and vegetation. Furthermore, the potential use of GRACE is expanded by applying innovative and exciting new methods of using the data. Aside from the findings pertaining to moisture-vegetation interactions, the developments in GRACE processing could be used by the general scientific community in areas not studied in this PhD, significantly contributing to future studies in this field of research. The three studies in this PhDd contribute to the wider scientific community by (i) developing a method to partition GRACE into shallow and deep subsurface storage. GRACE provides total water storage estimates that have no vertical definition. By decomposing GRACE into different temporal frequencies and comparing to a reference model, new shallow and deep estimations are created. This adds a new dimension of practicality to GRACE, a useful contribution towards large scale moisture estimations at different depths. (ii) Developing a method to reveal the moisture dependence of vegetation cover across different land use types. Previously, precipitation, soil moisture and GRACE have been used as indicators of the vegetation index. In this study, decomposed components of GRACE are used instead. This provides a comprehensive insight as to how vegetation responds to changes in moisture availability over different temporal scales, contributing to an understanding of how different events that lead to changes in moisture storage (i.e. drought) might affect vegetation. (iii) Demonstrating that biomass production is driven by dynamic water storage in water limited environments. The annual amplitude of GRACE is used to represent dynamic water storage, further contributing and extending methods in which GRACE can be used. Overall the scientific results of this thesis contribute towards future predictions of carbon fluxes and vegetation dynamics.

1.4 Review of Literature

Total water storage data from GRACE has become very popular in recent years and has been used in many studies. One notable use is the ability to monitor groundwater depletion over large spatial areas, e.g. large parts of India are shown to suffer from overexploitation (Rodell et al., 2009). Another example is how GRACE data has been combined with field measurements and models to assess hydrological conditions in Southeast Australia during the Millennium drought in the 2000s (Leblanc et al., 2009). GRACE data is also sometimes used in conjunction with other remote sensing products such as precipitation of the Tropical Rainfall Measuring Mission (TRMM) and vapotranspiration (NDVI) of the Moderate Image Resolution Spectroradiometer (MODIS) (Wang et al., 2014). It has been used to link terrestrial water to surface greenness by comparison to NDVI (Yang et al., 2014) and is used frequently to analyse precipitation (Chappell et al., 2013) (Peña-Arancibia et al., 2013). GRACE also presents a new way to measure evapotranspiration, which is usually only measured or modelled on a very small scale (Glenn et al., 2011). Finally, it has recently been used to gauge ice melt and sea level rise (Chen et al., 2013).

A potential limitation of GRACE is it's inability to directly estimate where water is stored in the vertical profile. The ability to do this is potentially extremely useful when studying large scale interactions between water and vegetation production. GRACE TWS estimates are given as the sum of all water in a given area. Numerous studies have used GRACE in conjunction with other data sources or model outputs to create new water storage estimates for a single component such as groundwater or soil moisture. Feng et al. (2013), Long et al. (2016) and Rodell et al. (2006) all estimate groundwater storage by subtracting modelled soil moisture and/or surface water estimates from GRACE TWS. A similar approach is conducted by Famiglietti et al. (2011), Leblanc et al., (2009), Swenson et al. (2008) and Yeh et al. (2006) who subtract in situ measurements of groundwater or soil moisture data from GRACE TWS to estimate the residual soil moisture or groundwater component. The use of assimilation techniques, where GRACE is combined within land surface models has also been used to estimate outputs of water storage at different vertical levels. Syed et al. (2008), Reager et al. (2015), Houborg et al. (2012) and Long et al. (2016) use such assimilation techniques, most commonly combining GRACE TWS estimates with NOAH land surface models to create new outputs of water storage at different vertical components. Due to the potential for in situ data to be scarce and expensive, and models to be unreliable or largely assumption based, there is a need for reliable estimates of various water storage components that have little or no dependence on field data or model outputs. A solution to this gap in knowledge is presented in chapter 2 of this thesis.

Changes in water storage in different storage reservoirs can lead to changes in vegetation mass and greenness (Yang et al., 2014). As water resources change as a result of natural and anthropogenic influences, it is increasingly important to understand how changes in terrestrial moisture affect biomass production. Previous studies have used different hydrological parameters to examine the effect of hydrological changes on ecosystem performance. Precipitation and soil moisture have most commonly been used to represent vegetation health and/production (Chen et al., 2014, Huxman, 2004, Méndez-Barroso et al, 2009, Wang et al., 2007). Both have shown generally meaningful correlations with ecosystem performance (by various measures such as Normalised Difference Vegetation Index (NDVI) and above-ground net primary production), but both indicators have demonstrated limitations. Not all precipitation is necessarily used by vegetation in an ecosystem. Some precipitation is lost from the ecosystem as runoff or soil evaporation (Liping et al., 1994). Only the part which is retained as soil moisture in the root zone can be consumed by vegetation (Bos et al., 2009). Soil moisture better represents the water that becomes available to vegetation. However, in situ soil moisture data is generally limited, spatially (vertically and horizontally) sparse and expensive, and estimations from land surface models are often highly uncertain (Chen et al., 2013). Yang et al. (2014) used monthly total water storage anomalies from GRACE to examine hydrological controls on variability in surface vegetation (NDVI), finding that GRACE a good indicator of seasonal variability in surface greenness over mainland Australia. These previous large-scale studies of interactions between terrestrial water storage and vegetation do not present how regions of different vegetation types are influenced by water storage changing at different temporal frequencies. This knowledge gap is addressed in chapter 3, using an extension of the method presented in chapter two.

Studies of interactions between terrestrial water storage and vegetation dynamics flow nicely into those concerning gross terrestrial primary productivity (GPP). Beer et al. (2010) show how GPP is well correlated to water fluxes, mediated by the vapour pressure deficit in forested regions of Europe. Zhao et al. (2010) find a reduction in GPP during droughts in the southern hemisphere from 2002-2009, and Ciais et al. (2003) report reductions in GPP during extreme heat and drought in Europe. Based on modelling, Tian et al. (2010) report increases in GPP which correlate with water use efficiency in the United States of America and models by Churkina et al. (1999) demonstrate a strong relationship between water availability and GPP that is altered when other environmental conditions are considered. GPP and annual precipitation have a linear relationship, mostly accounted for by grasses according to Yahdjian et al. (2006) in Argentina. These previous studies show different drivers of ecosystem performance in the areas in which they are conducted. None of which explore the global driver of ecosystem performance specifically in water limited ecosystems, or use data such as GRACE to compare with local and or global GPP information. This knowledge gap is addressed in chapter 4, by comparing dynamic water storage, represented by annual water storage amplitude, to GPP estimations from a remote sensing database (MODIS).

The chapters in this thesis address gaps in knowledge relating to large scale interactions between terrestrial water stores and ecosystem production, as well as the development of methods to expand the usefulness of GRACE. The chapters are linked as they progress, with a method developed in chapter 2 being applied in chapter 3, and further advances in water and ecosystem relations using GRACE being made in chapter 4. The gaps in knowledge which are filled in this thesis contribute towards future predictions of carbon fluxes vegetation dynamics and the extended potential of GRACE.

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1.5 Recurring data and methodologies

The studies presented in chapters 2,3 and 4 of this thesis use data and methods that in some cases overlap between chapters. A brief overview of those data and methods used in more than one chapter is presented below, not including specific processing details for each chapter.

1.5.1 GRACE data (chapters 2, 3 and 4)

In each chapter of this thesis, GRACE total water storage data is used. It was freely downloaded from the GRACE Tellus website (http://grace.csr.nasa.gov/data/get-data/). GRACE data is available from different institutions, in this thesis it is from the University of Texas's Centre for Space Research (CSR) and NASA's Jet Propulsion Laboratory (JPL). In all cases the recommended scaling coefficients were applied to GRACE data (Swenson & Wahr, 2006), which are designed to remove leakage errors and do so significantly (Landerer & Swenson, 2012). Although not the true resolution of GRACE, we use data presented spatially in 100 km by 100 km cells. This resolution is obtained using the NOAH land surface model in conjunction with de-striping and scaling filters, deeming the 100km x 100km accurate and suitable for use.

Where a month of data is missing in the GRACE data set, estimations are created 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).

1.5.2 Wavelet decomposition (chapters 2 and 3)

Wavelet decomposition is a method of extracting multiple time series of data from a single time series. The method expresses decompositions as a multitude of smaller 'waves' at different temporal frequencies (He et al., 2013). In this thesis, the Meyer wavelet is used to decompose

GRACE TWS into components at different temporal. This is achieved by means of a MATLAB code using the 'wavdec' function. Data are decomposed into different '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… and D1, D2, D3… for approximations and details respectively, with the time scale increasing with the decomposition number e.g. for monthly data A1/D1 (2-month scale), A2/D2 (4-month scale), A3/D3 (8-month scale) and A4/D4 (16-month scale). In chapters 2 and 3 of this thesis, four decomposition 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, 4 details and 4 approximations. These decompositions are analysed against water storage estimates and vegetation cover/greenness.

1.5.3 Stepwise regression (chapters 2 and 3)

A stepwise regression is a process where by predictor variables, such as decomposed GRACE TWS frequencies that fit within a single dependant variable, such as model estimates of TWS are automatically selected. This selection is made based on the p-value of the predictor variable being less than 0.05. When the studies in this thesis use a stepwise regression it was performed with the 'stepwise' fit function in Matlab. Data and time series selected by the stepwise regression are used to create new estimates of TWS or vegetation dynamics, depending on the study.

2. Estimation of GRACE Water Storage Components by Temporal Decomposition

2.1 Abstract

The Gravity Recovery and Climate Experiment (GRACE) has been in operation since 2002. It provides total water storage estimates globally for cells sized roughly 100 km by 100 km. Mapping 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

2.2 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 (2016) due to its success in hydrological and other applications. 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 total of all water stored in a GRACE cell, regardless of its type, i.e. surface water, soil water, groundwater and vegetation-bound water are all together in one TWS value (Rodell & Famiglietti, 2001). GRACE TWS data has become very popular in recent years and has been used in many studies. 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). A summary of relevant literature regarding the estimation of individual or multiple water storage for varying applications using GRACE TWS is presented in Table 2.1.

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 is no documented method to comprehensively 'split' GRACE data into multiple desired water storage components.

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 chapter, 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 2.1: 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
(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.
(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.
(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, 6,500,000 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.

2.3 Data

2.3.1 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 was suitably post-processed including applying the recommended scaling coefficients (Swenson & Wahr, 2006). The scaling coefficients are in part designed to remove leakage errors and do so significantly (Landerer & Swenson, 2012). We used the longest available monthly time series, from March 2003 to December 2014. The data are presented spatially in 100 km by 100 km 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).

2.3.2 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 on both remote sensing data and field observations. The model's documentation insists 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 (Vaze et al., 2013). 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 from the AWRA model 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.

2.3.3 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.

2.4. Methodology

2.4.1 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.

2.4.2 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, **$S_{shallow}$ (S0 + Ss)** and **S_{deep} (Sd+Sg).**

2.4.3 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. For this test an 8 level Meyer decomposition was used. 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.

2.4.4 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.

2.4.5 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 calculated equation 2.1 with the selected predictor variables.

$$Y = \beta_0 + \beta_i X_i \ldots + \varepsilon \tag{2.1}$$

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 2.2,

$$E = 1.0 - \frac{\sum_{i=1}^{N}(O_i - P_i)^2}{\sum_{i=1}^{N}(O_i - \bar{O}_i)^2} \tag{2.2}$$

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.

2.5. Results

2.5.1 Concept demonstration

Figure 2.1 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.

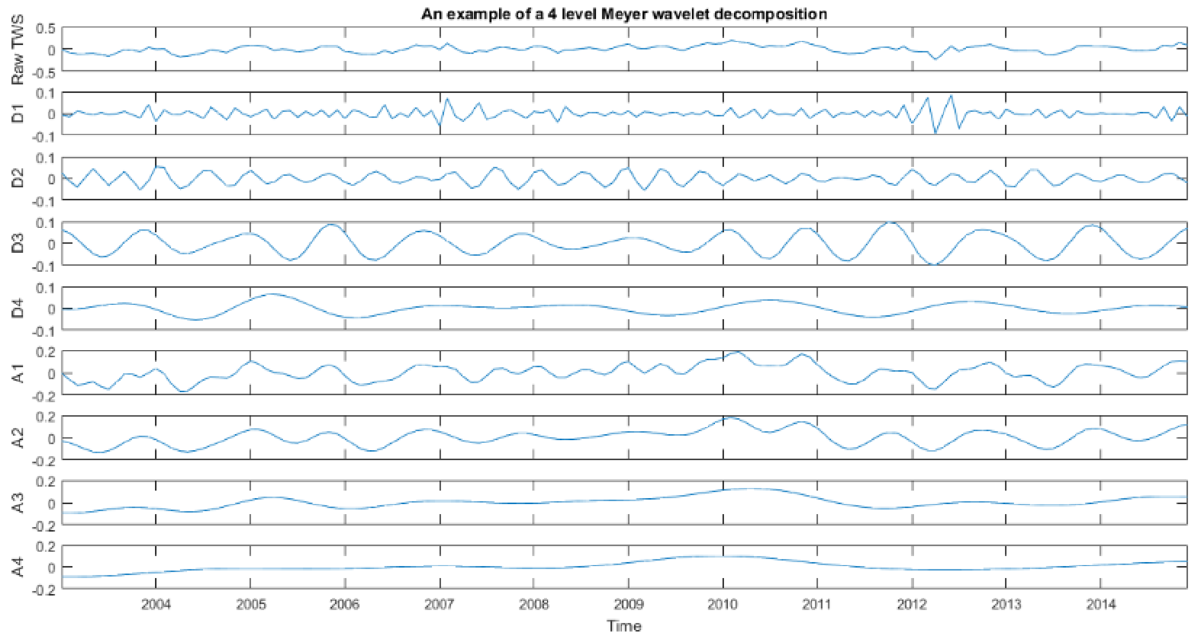

Figure 2.1: An example of a wavelet decomposition from the western-most cell in Australia (S 23.5°, E113.5°). Notice the visible trends in the approximations, which are normalised in the details.

A test of the method using soil moisture data from Aldinga Scrub demonstrates the improvement to estimations that can made using the method (Figure 2.2). 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.

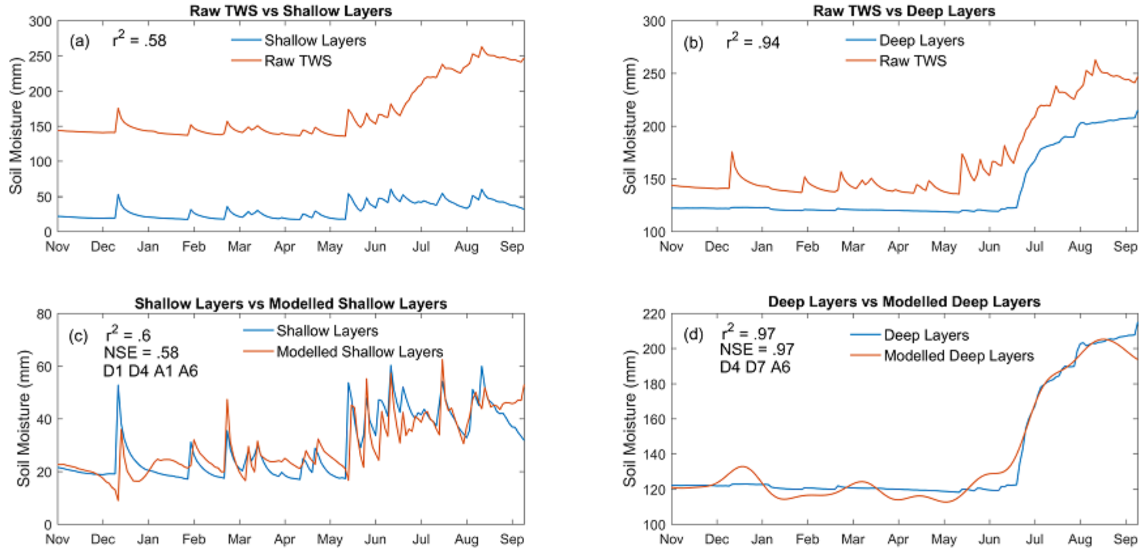

Figure 2.2: Results using the wavelet decomposition and stepwise regression method for estimates of soil moisture at different depths. Plots a and b show the soil TWS vs the shallow and deep layers. Plots c and d show the estimations of the shallow and deep soil layers. The r^2 value is increased using 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. 2.3). The R^2 values increased for all cells, while a few cells 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.

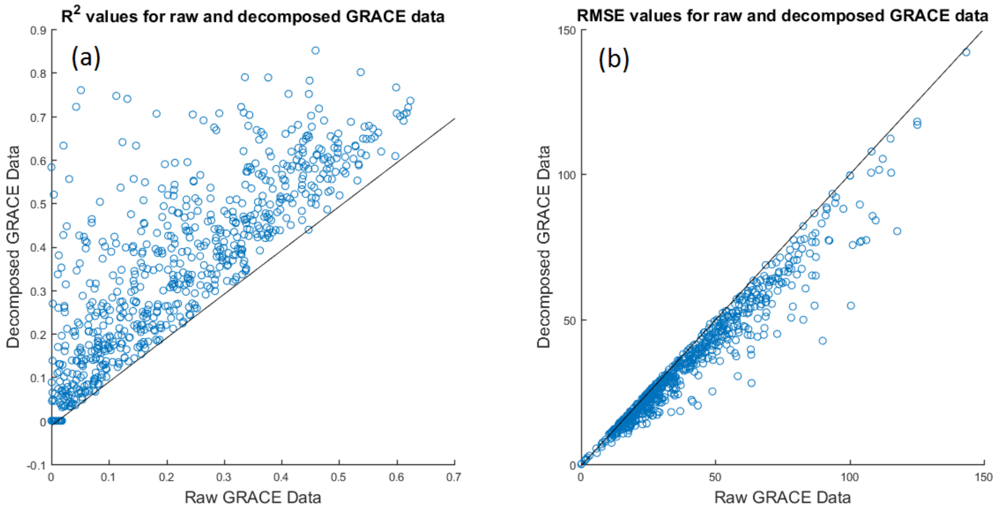

Figure 2.3: (a) results from the proof of concept test. R^2 values for estimations of all water storage components using raw GRACE data vs R^2 values for estimations of all water storage components using decomposed GRACE data. (b) RMSE for estimations of all water storage components using raw GRACE data 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.

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 version 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 2.4). Again, at this stage the storage components are not split and the result simply further demonstrates the concept and ability of the method.

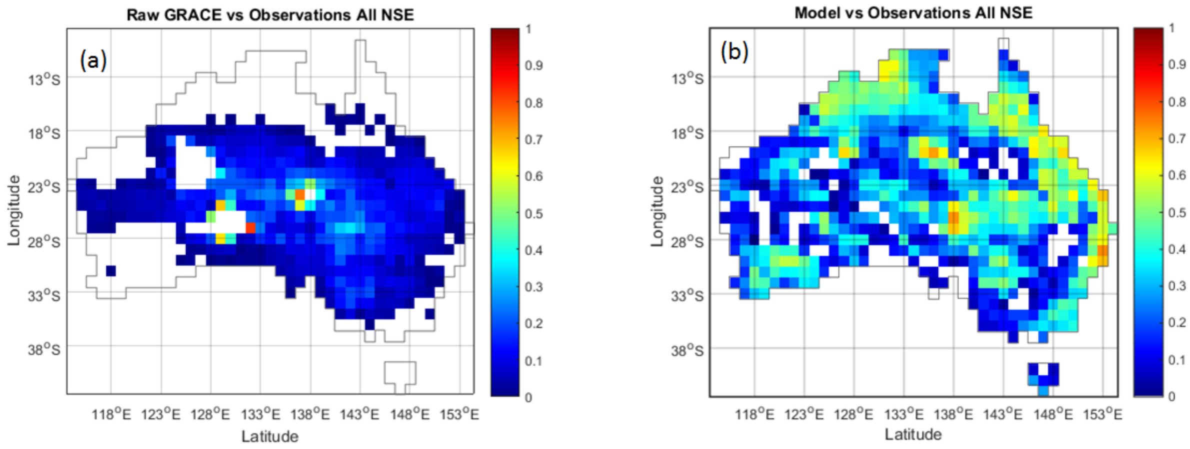

Figure 2.4: (a) NSE values for raw GRACE data compared to the sum of all four AWRA model water storage components. The results are generally poor with few values above 0 and many negative NSEs (depicted by white cells within the boundary). (b) NSE values for the sum of all decomposed GRACE values compared to the sum of all four AWRA model values. The results are well improved with higher values across the continent and fewer negative NSEs.

2.5.2 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 2.5). 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.

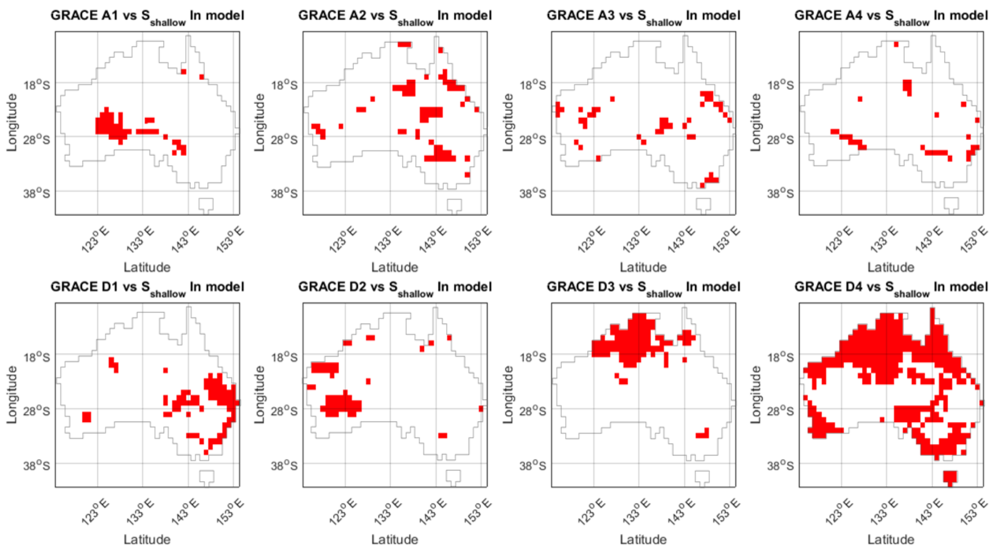

Figure 2.5: For each GRACE decomposition the cells (in red) are highlighted that are included in the stepwise regressions for the estimation of $S_{shallow}$. Although spatially varying the most important variables are D4, followed by D3 and D1.

The comparison between the estimated $S_{shallow}$ storage component and the shallow storage of the AWRA model shows a wide range of NSEs across the continent, from average, slightly above 0, to very good, above 0.9 (Figure 2.6). Areas with high NSEs are observed in the northern most part of the continent, the south west corner of Western Australia and most of the coastal fringe. NSEs 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.

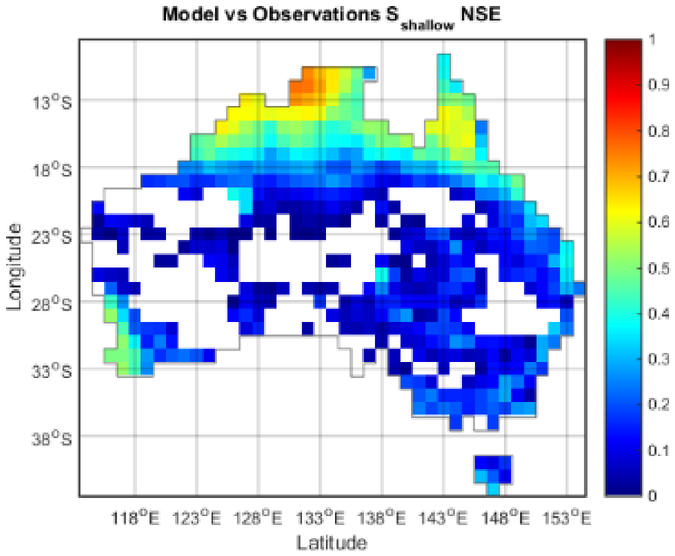

Figure 2.6: Nash Sutcliffe efficiencies for each cell for the $S_{shallow}$ estimation compared to the AWRA model. Results show strong spatial structure with the highest NSEs located in the north, south west and scattered throughout the east of the continent. NSEs equal to or less than zero are depicted by white cells within the boundary.

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 2.7). 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 cells 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.

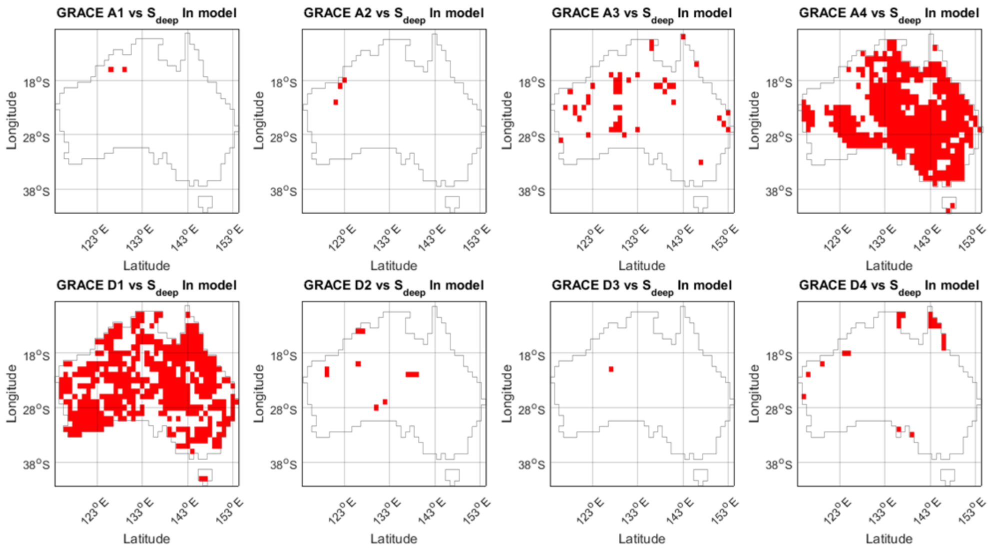

Figure 2.7: Cells for each variable that are selected for the estimations of S_{deep} by stepwise regressions are highlighted in red. For S_{deep} there is a very strong, continent-wide inclusion of A4 and D1 as well as an interesting inclusion of D4 almost exclusively around the coast.

S_{deep} also shows a range of spatially varying NSEs ranging from average to very good (Figure 2. 8). There is a very large cluster of high NSEs 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 NSEs are lower, there are a minimal number of cells with a negative NSE, meaning the estimation's performance is still good overall.

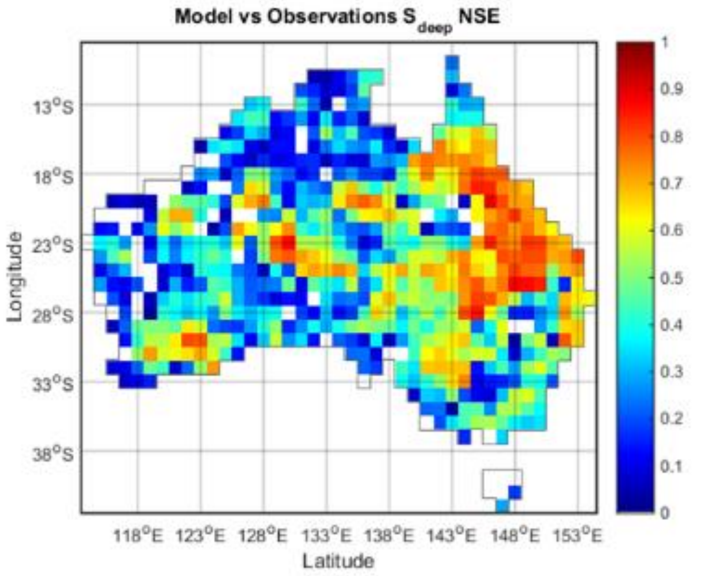

Figure 2.8: Nash Sutcliffe Efficiencies for each cell for the comparison of the S_{deep} estimations versus the AWRA model. Results are best through the Great Artesian Basin, South-Western Australia and central parts of the continent. NSEs equal to or less than zero are depicted by white cells within the boundary.

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 cells 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.

2.6. 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 NSEs 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 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. While all of these studies show promising results, the quality is limited 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.

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. 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.

2.7. 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 for each cell 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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3. Large-scale vegetation responses to terrestrial moisture storage changes

3.1 Abstract

The Normalised Difference Vegetation Index (NDVI) is a useful tool for studying vegetation activity and ecosystem performance at a large spatial scale. In this study we use the Gravity Recovery and Climate Experiment (GRACE) total water storage (TWS) estimates to examine temporal variability of NDVI across Australia. We aim to demonstrate a new method that reveals the moisture dependence of vegetation cover at different temporal resolutions. Time series of monthly GRACE TWS anomalies are decomposed into different temporal frequencies using a discrete wavelet transform and analysed against time series of NDVI anomalies in a stepwise regression. Results show that combinations of different frequencies of decomposed GRACE TWS data explain NDVI temporal variations better than raw GRACE TWS alone. Generally, NDVI appears to be more sensitive to inter-annual changes in water storage than shorter changes, though grassland-dominated areas are sensitive to higher frequencies of water storage changes. Different types of vegetation, defined by areas of land use type show distinct differences in how they respond to the changes in water storage which is generally consistent with our physical understanding. This unique method provides useful insight into how NDVI is affected by changes in water storage at different temporal scales across land use types.

Key words: Vegetation index, NDVI, GRACE, ecosystem performance, water storage, wavelet analysis, regression analysis, land use type

3.2 Introduction

In many parts of the world, such as Australia, water storage is the dominant limiting factor in vegetation growth (Donohue et al., 2008). As such, changes in water storage can lead to changes in vegetation mass and greenness (Yang et al., 2014). As vegetation plays a vital role in gross primary production and the carbon and hydrological cycles, studies of the temporal and spatial variation of vegetation are vital for understanding ecosystem performance and its climatic responses (Campos et al., 2013). As the climate and water resources change as a result of natural and anthropogenic influences, understanding how fluctuations in water storage is associated with biomass changes can have profound importance in the future.

Previous studies have used different hydrological parameters to examine the effect of hydrological changes on ecosystem performance. Most commonly, precipitation and soil moisture have been used as defining variables (Chen et al., 2014, Huxman, 2004, Méndez-Barroso et al, 2009, Wang et al., 2007). Both of these have shown generally meaningful correlations with ecosystem performance (by various measures such as Normalised Difference Vegetation Index (NDVI) and above-ground net primary production). However, both indicators have shown limitations. The total amount of precipitation is not necessarily used by vegetation in an ecosystem. Part of precipitation is lost from the ecosystem as runoff or soil evaporation (Liping et al., 1994). Only the part which is retained as soil moisture in the root zone can be viably consumed by vegetation, categorised as 'effective precipitation' (Bos et al., 2009). For a given amount of rainfall the fraction of effective precipitation varies spatially due to differing geographical features, soil types, and vegetation cover conditions. Soil moisture gives a better representation of the water that becomes available to plants. However, in situ soil moisture data is generally limited and spatially (vertically and horizontally) sparse. Estimations from land surface models are often highly uncertain (Chen et al., 2013).

More recently Yang et al. (2014) used monthly total water storage anomalies (TWS*) from the Gravity Recovery and Climate Experiment (GRACE) to examine hydrological controls on variability in surface vegetation. GRACE provides monthly global terrestrial water storage derived from variations in the earth's gravity field. The authors suggested that where large surface water reservoirs do not exist, GRACE TWS changes are mostly from soil moisture and groundwater, making it ideal for examining hydrological controls on vegetation activity. GRACE is found to be a good indicator of seasonal variability in surface greenness over mainland Australia (Yang et al., 2014). For the period 2003-2010, for which GRACE data is available, changes in NDVI* are explained more strongly by GRACE TWS* than by precipitation, suggesting it poses a more direct influence on surface greenness and ecosystem performance.

GRACE TWS gives the total relative water storage per 100 km by 100 km cell. This is the sum of surface water, soil water, groundwater, ice and other reservoirs. We previously developed an approach to 'split' GRACE TWS into shallow and deep subsurface storage components using discrete wavelet decomposition (Andrew et al., 2016). In this study, we aim to expand on the general findings of Yang et al. (2014) by decomposing GRACE TWS* into different temporal components and analysing them against NDVI*. Given that root zone water storage is the source of water to vegetation we hypothesize that decomposed TWS* data that reflects the temporal patterns of the root zone will perform better than the total TWS* in association with NDVI*.

The questions we seek to address are (1) does the decomposed TWS* data show a better relationship to NDVI* than the 'raw' TWS* data; (2) how does the sensitivity of NDVI* in response to changes in TWS* vary spatially; and (3) which temporal components of TWS* are most significant in influencing NDVI* for different land use types across Australia.

3.3 Data

3.3.1 GRACE data

GRACE total water storage (TWS) data from The University of Texas Centre for Space Research (CSR), and NASA's Jet Propulsion Laboratory (JPL) are used. The gridded data were freely downloaded from the GRACE Tellus website (http://grace.jpl.nasa.gov/data/get-data/). We use the provided scaling coefficients to process the data as recommended by Swenson and Wahr, (2006). The scaling coefficients are in part designed to remove leakage errors (Landerer and Swenson, 2012). Monthly data from March 2003 to December 2014 is used. The average of the two data sets is calculated for each cell at each month to reduce the uncertainty. The data is presented spatially in 100 km by 100 km grid cells. Cells which are used in the study are selected based on their comparison to a shapefile of Australia. For a coastal cell to be included it had to have been covered at least two thirds by land mass such that noise from the ocean did not alter the analysis.

In some instances, a month of GRACE data is missing. Where this occurs, the missing data are filled with a simple temporal interpolation using the months either side. Because of the monthly temporal resolution this is deemed appropriate and maintains the average seasonal cycle well (Long et al., 2015).

3.3.2 NDVI data

We use GIMMS 3g NDVI data for the same time period as the GRACE data. The data is downloaded from the NASA database. The NDVI data is produced at a smaller spatial scale (.25 by .25 degrees) than GRACE. They are rescaled to match the GRACE cell size using the resampling tool in ArcGIS. Like the GRACE data, only cells which contain at least two thirds land are used, and missing data are filled by a temporal interpolation.

3.3.3 Land Use Type data

The moderate-resolution imaging spectroradiometer (MODIS) land use data from 2012 is used to identify different land use types across Australia. It is freely available online from http://glcf.umd.edu/data/lc/. In regards to rescaling and cell selection, the same procedures are applied as in the case of NDVI data. In Australia, MODIS land use type data defines 12 different classes of land use. This is reduced to five (or six including barren land) classes by grouping similar classes such as different types of forests. The resulting land use types are: forest, shrubland, savanna, grassland, and agricultural land (Table 3.1).

Table 3.1: Subcategories of land use types as defined by MODIS

MODIS Land Use Type	**Classification in this study**
Evergreen needle leaf forest Evergreen broad leaf forest Deciduous needle leaf forest Deciduous broad leaf forest	*Forest*
Closed shrublands Open shrublands	*Shrubland*
Woody savanas Savanas	*Savana*
Grassland	*Grassland*
Cropland Cropland/Natural vegetation mosaic	*Agricultural land*
Barren	*Barren*

Figure 3.1 shows the spatial distribution of different land use types across Australia, grouped as previously stated (Table 3.1). Note no analysis is performed for areas considered barren, due to a lack of vegetation.

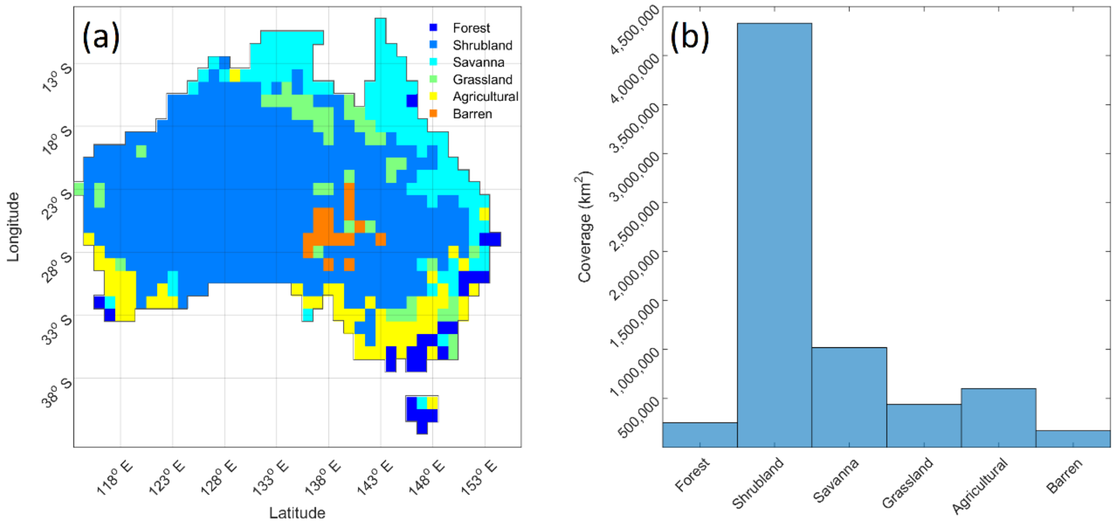

Figure 3.1: (a) The spatial distribution of various land use types across Australia and (b) the area covered by each land use type.

3.4 Methodology

3.4.1 Calculating anomalies

For variables with strong seasonality, a statistical relationship between them does not necessarily mean a physical relationship exists. Climatological anomalies of both GRACE TWS and NDVI are used in order to remove seasonality in the data which would otherwise result in large, but irrelevant and misleading correlations between variables examined in this study.

The anomalies are calculated following the method of Yang et al. (2014), as shown in Equation. (3.1).

$$X'(i,j) = X(i,j) - \frac{1}{n}\sum_{j=1}^{n} X(i,j) \qquad (3.1)$$

where X^* represents the climatological anomaly of X (i.e. raw GRACE TWS), i is the month, j is the year and n is the total number of years.

New lagged GRACE TWS* anomaly data sets are produced by offsetting the GRACE data from the NDVI data by one to six months. This is to allow any delays in NDVI response to water storage to be revealed (Farrar et al., 1994).

3.4.2 Wavelet decomposition

GRACE TWS* is decomposed into different signals using a discrete wavelet transform. Introduced in the early 1980s, a wavelet is a mathematical function used to divide data series into different-frequency components (Goupillaud et al., 1984). The method expresses decompositions as a multitude of smaller 'waves' at different frequencies (He et al., 2013). In this study we use the Meyer wavelet to decompose GRACE TWS* into different temporal components which is suitable for this temporal data (He & Guan, 2013). This is achieved using the 'wavdec' function in Matlab. Data is decomposed into 'approximation' and 'detail' components that each represent the data at its different temporal scales. Detail series neglect trends while approximation series maintain trends in the data (Nalley et al., 2012). The resulting time series are labelled A1, A2, A3, A4 and D1, D2, D3 D4 for approximations and details respectively. The temporal scale increases with the decomposition level e.g. A1/D1 (2-month scale), A2/D2 (4-month scale), A3/D3 (8-month scale) and A4/D4 (16-month scale) (Figure 3.2).

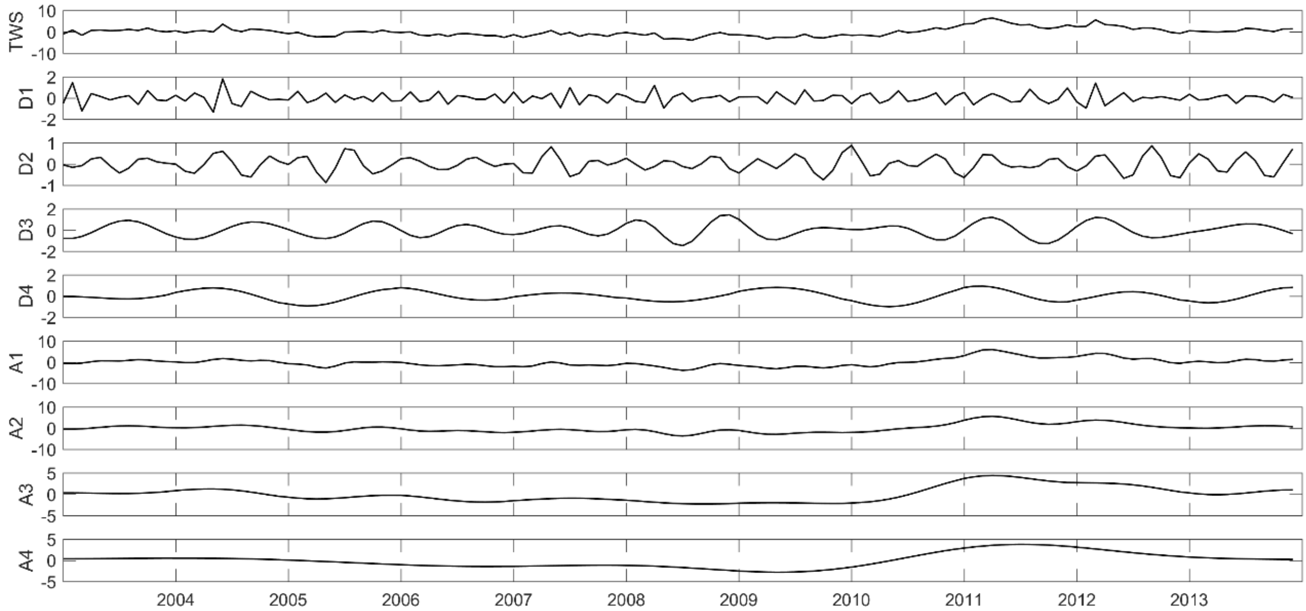

Figure 3.2: An example of a wavelet decomposition from a cell in central South Australia (29°S 136°E). Notice the visible trends in the approximations, which are normalised in the details.

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 is too coarse for a time series of only 11 years of raw data. Because all but the lowest approximation levels contribute partly to details, we only use the lowest frequency approximation, along with all of the details. The sum of these (D1, D2, D3, D4, A4) equals the raw signal (Figure 3.3). So, five wavelet decomposition series are produced for GRACE data as well as each of the six lagged series' for each decomposition level giving a total of 35 water storage time series.

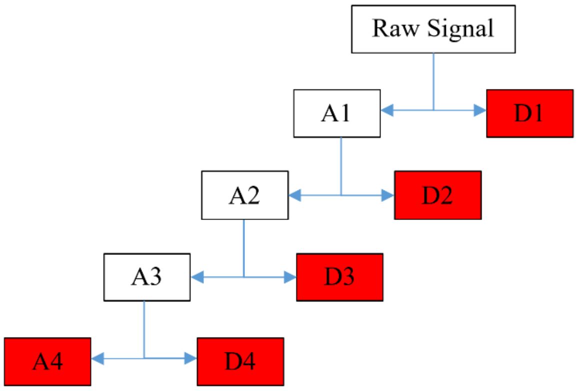

Figure 3.3: The structure of a wavelet decomposition; decomposition levels used in this study are highlighted in red.

3.4.3 Stepwise regression

We used a stepwise regression for every cell with NDVI* as the dependant variable and the GRACE TWS* decompositions as predictor variables. Given the time series of the data, 35 predictor variables is too many for a stepwise regression to function properly. The stepwise regression is run multiple times and the best predictor variables are chosen narrowing them down to nine. The choice is made based on the amount of cells selected for each variable from the stepwise regression and how relevant they are given their spatial coherence. In general, the predictor variables excluded from the stepwise regression are not included in any cells across the country. The remaining variables are (subscript denotes lag in months) $D1_0$, $D2_1$, $D3_0$, $D3_1$, $D3_2$, $D4_0$, $D4_1$, $A4_0$, and $A4_6$.

3.5 Results

As a proof of concept, the relationships between raw GRACE TWS* and NDVI*, and decomposed GRACE TWS* and NDVI* are compared (Figure 3.4). The results for the decomposed TWS* data are based on a selection of decomposed time series selected by the stepwise regression. A time series example of the results from an individual cell demonstrated in figure 3.5. For each cell the correlation coefficient between NDVI* and the regression estimates (*r*) is calculated. In order for the tests to be comparable, lagged data is not included in the decomposed TWS dataset for this demonstration, it shows purely how decomposed data improves the relationship. A scatter of the r values shows a clear improvement in the relationship when decomposed GRACE TWS* data is used as opposed to raw, with all points above the 1:1 line. Student-t tests confirmed that the stepwise regression results are statistically highly significant with a t-statistic p value of respectively 2.3 and .00014.

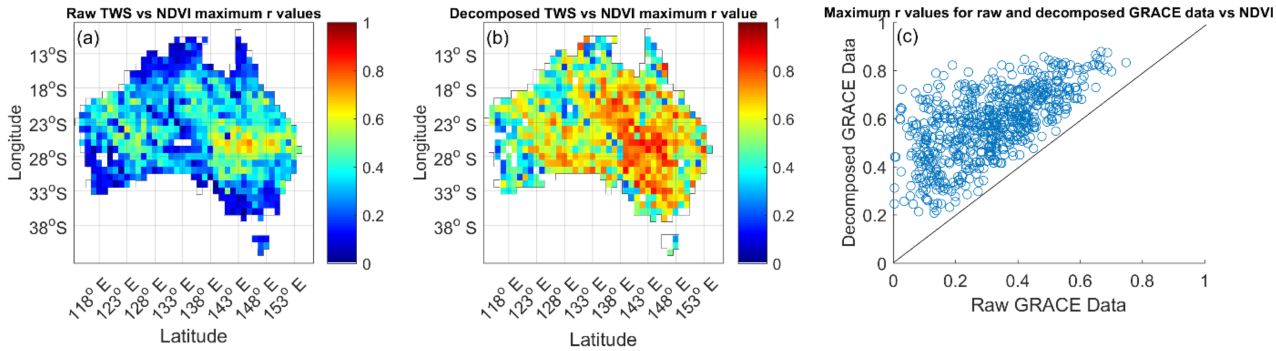

Figure 3.4: (a) The *r* values using raw TWS* and NDVI*. (b)The r values using decomposed TWS* and NDVI*. (c) a scatter of the results shows a clear improvement in the relationship when decomposed data is used.

Lagged data ensures the relationship between NDVI* and TWS* is well represented, but the decomposed frequency of the TWS* data is the focus in this study. Though the stepwise regression is performed using nine variables including lags where suitable, the results herein are presented as only five variables, D1, D2, $D3_L$, $D4_L$ and $A4_L$. For each detail or approximation level using different lags, one variable is created by combining the results of different lagged data sets together to present the results i.e. $D3_L = D3_0+D3_1+D3_2$.

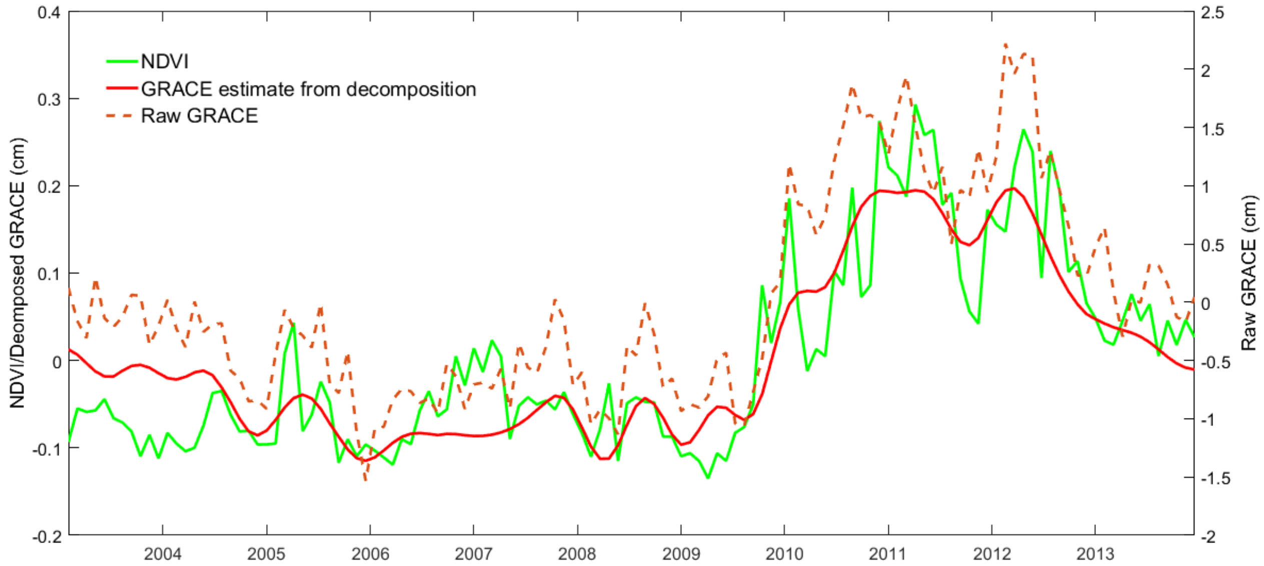

Figure 3.5. An example of the time series from a single cell. The new estimate uses the coefficients from A40, A46 and D4 as chosen by the stepwise regression. Pearsons coefficient (r) between the decomposed GRACE estimate and NDVI* is 0.872, compared with 0.665 when using raw GRACE TWS*.

It is important to recognise how the variables that are included in the stepwise regression vary spatially to understand how vegetation responds to different temporal patterns water storage across the continent. For a variable to be included in the stepwise regression it does not have to show a positive correlation. Figure 3.6 shows which variables are included in the regression for each cell across Australia. Where no lagged data is used (D1 and D2) the colour denotes whether the coefficient is positive or negative. Where lagged data is used ($D3_L$, $D4_L$ and $A4_L$) the colour denotes whether all coefficients for a cell had the same -/+ sign or not. Figure 3.6 shows that while $A4_L$ is included across most of the country, one of the lagged data sets, $A4_6$ has a large amount of negative coefficients included in the regression (see appendix 3A). A possible explanation for this is that NDVI is susceptible to the 'memory effect', where past inputs and outputs affect responses in the system (Shook & Pomeroy, 2011).

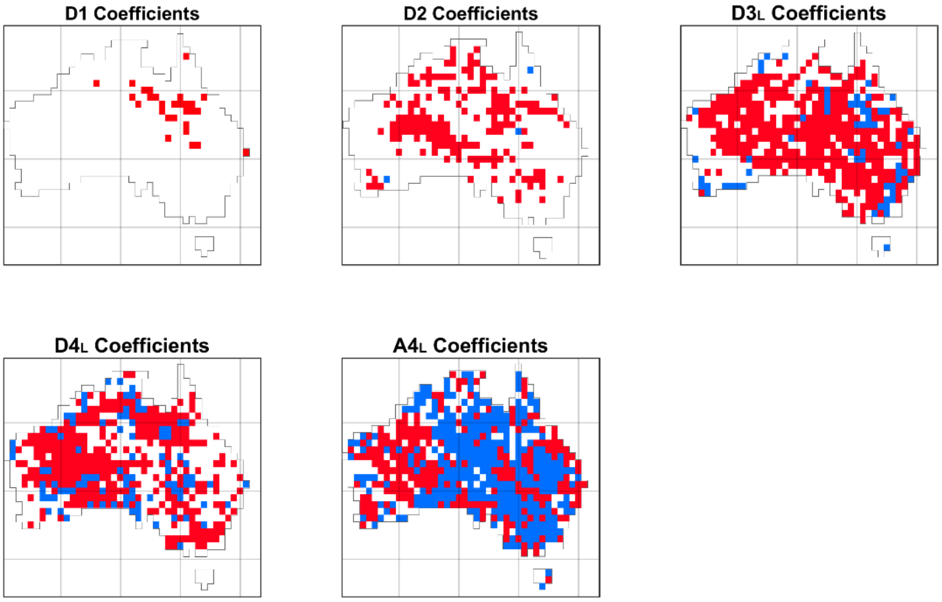

Figure 3.6: Coefficients for each decomposition level. For D1 and D2 no lags are used, red represents for these a positive coefficient and blue represents a negative coefficient. For D3$_L$, D4$_L$ and A4$_L$ (which include lags), red represents cells where all coefficients are positive. Blue represents cells where at least one lag had a negative coefficient.

Overall, the number of cells covered by each different decomposition level increases as the decomposition time scale increases. This shows that in general, NDVI changes pertain to longer time-scale water storage changes and is not affected as much by changes on monthly time scale.

While understanding which variables are used in each cell is important, it is more important to know their relative impact on NDVI*. The relative weight of each variable is calculated to show the importance of each on vegetation in different land use types. Of the included variables in each cell, the relative weight of each variable is calculated using Equation (3.2).

$$W = \frac{(C \cdot \sigma_X)}{\sigma_{NDVI}} \tag{3.2}$$

Where W is the relative weight, C is the coefficient, σ_X is the standard deviation of the decomposed data anomaly (X), σ_{NDVI} is the standard deviation of the NDVI anomaly. Figure 3.7 shows which variable has the highest relative weight in each cell. $A4_L$ is the dominant variable, covering the majority of the country, and is a low frequency trended signal. D2, a higher frequency signal is the second most dominant variable and shows generally clear spatial coherence.

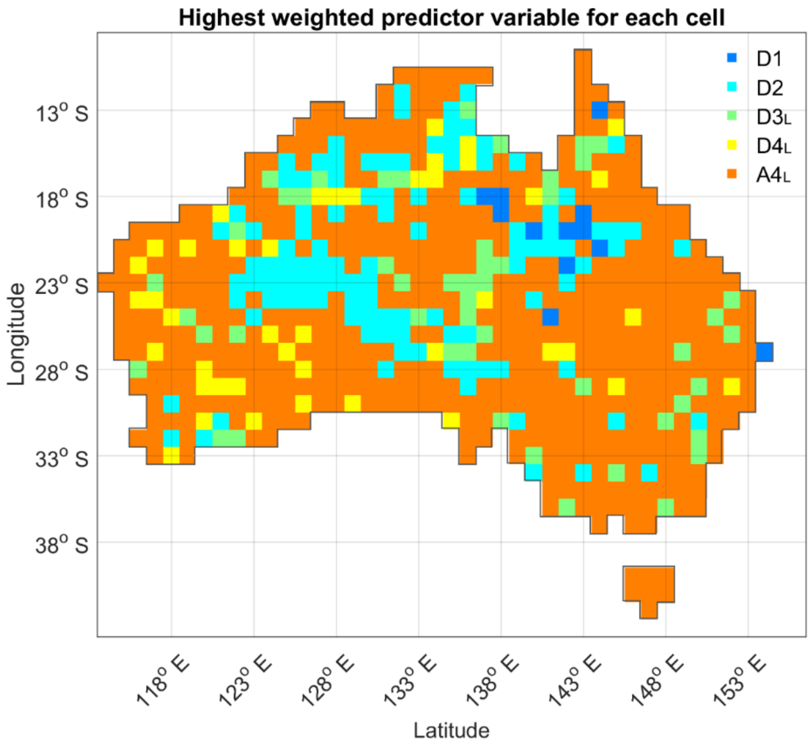

Figure 3.7: The variable with the highest relative weight in the regression for each cell across Australia. A4 is most dominant, however D2 is prominent in distinct areas throughout central Australia. D1, $D3_L$ and $D4_L$ all occur but with little spatial coherence.

The relative weights for all cells of each land use type are combined and presented as a relative weight percentage per land use type (Figure 3.8).

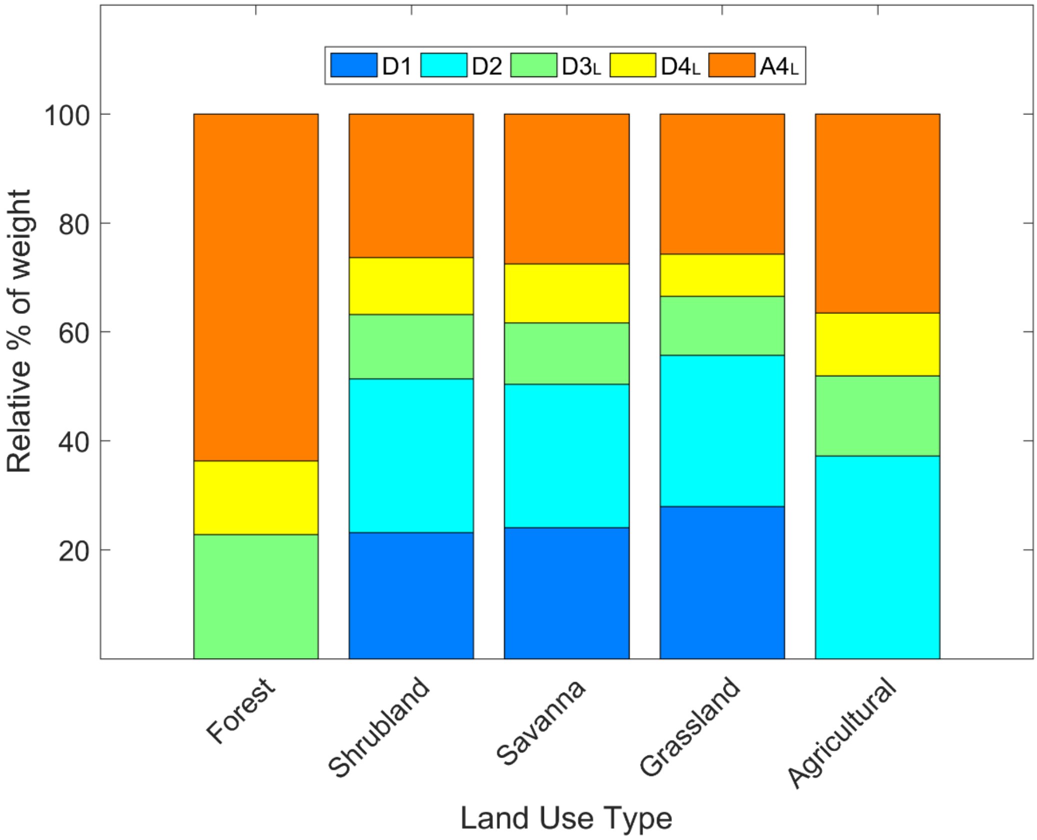

Figure 3.8: The relative weight of each decomposed TWS* for each land use type. Forests are $A4_L$ dominated, shrublands, savannas and grasslands are very similar with relative equal weights of D1, D2 and $A4_L$, while agricultural land is dominated by D2 and $A4_L$.

Forested areas have only low frequency decompositions included, with $A4_L$ being the most dominant. This is expected as forests have deep root systems which tap into water stores which change slower than shallower water (Backer et al., 2003). Therefore, their water availability is less likely to be affected by short-term rainfall or evaporation, relying more on long term hydrological trends. Shrubland, savanna and grassland show nearly identical distributions of weights. Grassland shows a marginally higher percentage of the D1 and D2 variables, which is consistent with our physical understanding as they are fed by shallow soil moisture which varies at a short time frequencies. While all are defined differently, the three land use types have overlapping characteristics, most commonly the widespread presence of short grasses (Friedl et al., 2002) and shallow root systems. These short grasses respond to changes in the shallow top layer of the soil which is influenced at high temporal frequencies by rainfall events and evaporation. The similarity in the result of these three land use types suggests that they are hardly distinguishable by GRACE, likely due to the spatial extend of GRACE cells. For example, where sparse trees exist in a savanna, their influence on the shallow soil moisture may be negligible compared to the large coverage of grasses, thus showing a very similar pattern to grassland.

3.6 Discussion

Using wavelet decomposed GRACE TWS* data proved to improve the correlation between water storage and NDVI*. A previous study by Yang et al. (2014) showed that GRACE is a superior indicator of surface greenness than soil moisture or precipitation, which were earlier used as indicators (Chen et al., 2014, Huxman, 2004). Temporal decomposition of GRACE TWS* produces a new temporal dimension that allows the data to be analysed to its full potential. As demonstrated in Figure 3.4, the decomposed TWS* data is better associated with the surface greenness than the raw TWS*. Furthermore a better understanding of how surface greenness changes with water storage spatially and temporally is achieved, with different levels of decomposition existing in spatial clusters across the country. The dominance of $A4_L$ as the most highly weighted predictor variable indicates that generally vegetation responds to low frequency (inter-annual) changes in water storage across Australia.

An interesting result is the large amount of negative coefficients produced from the stepwise regression for $A4_6$. Two possible explanations exist. A 6-month lag may correspond to the opposite seasons e.g. wet 6 months ago, dry now, potentially serving as an indicator of water storage potential. Alternatively, vegetative systems may be susceptible to the 'memory effect.' Specifically, this would suggest that for most of the continent, trends at the A4 scale (roughly annual) influences vegetation responses to water storage changes six months later in these areas. Such a memory effect can serve as an indicator of an ecosystem's capacity to store water, as well as carbon and nitrogen (Schwinning et al., 2004).

The weight distribution of different decompositions across land use types generally matches our physical understanding. Note firstly that all five land use types have $A4_L$ as a large component of their total weight. This is a further indication of the general response of vegetation to low frequency changes in water storage. Forested areas are only composed of $A4_L$, $D4_L$ and $D3_L$, irrelevant to high frequency changes in water storage. This matches our physical understanding as forests have deeper root systems which rely on seasonal changes or long term hydrological trends. Interestingly, shrublands, grasslands and savannas show a near identical composition of relatively weighted decompositions, with grasslands showing a slightly higher weight percentage of D1 and D2. The three land use types are all grass dominated, with the addition of sparse trees and shrubs in savannas and shrublands. As the resolution of GRACE cannot pick up these additions, it is possible that they all appear as grassland, or at least skewed that way, as that is the dominant vegetation cover. The dominance of D1 and D2 across these land use types is typical of relatively dynamic, grass dominated regions.

The combination of weights that make up the total for agricultural land is less straightforward. D2 and $A4_L$ contribute to large portions of the total. One major difference between agricultural land and the other land use types is the anthropogenic contributions to the land, including the additions of livestock grazing (Yates et al., 2000). The other land use types are generally self-sufficient/limiting at the cell scale, so the interruption of the natural cycle of the vegetation in agricultural areas is a potential anomaly, disturbing any predictable composition of relative weights.

Our method of using decomposed terrestrial water storage as an improved indicator of surface greenness has potential environmental benefits. It allows for an improved understanding of how vegetation responds to changes in water storage at a spatiotemporal level. This in turn serves as a better indicator of ecosystem performance and carbon fluxes. With predictions of terrestrial water storages to decline in the future (Gleick, 1989), the method could be highly useful for predicting carbon fluxes and ecosystem performance based on future water storage estimates. Furthermore, the global mapping of GRACE and NDVI (as well as other vegetation indexes) means that it could be applied globally.

3.7 Conclusion

In this study we aimed to increase the understanding of the links between GRACE TWS* and NDVI* by using a decomposed TWS* data. Combinations of decomposed GRACE TWS* data show an improved relationship with NDVI* than raw GRACE TWS* data alone. Varying decomposed frequencies show spatial coherence in parts of the country, sometimes independently and sometimes overlapping other decomposed frequencies. Generally, NDVI is influenced by low frequency changes in water storage; however there are some areas which are also sensitive to high frequency changes. NDVI is susceptible to a memory effect which depends on previous TWS conditions, 6 months generally. The total influence of NDVI changes is made up of storage changes over different time periods. These vary depending on the land use type and the results are aligned with our physical understanding. This analysis could be used further to continue to improve our understanding of vegetative responses to storage change in Australia and globally and benefit predictions of ecosystem performance and carbon fluxes.

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Appendix 3A

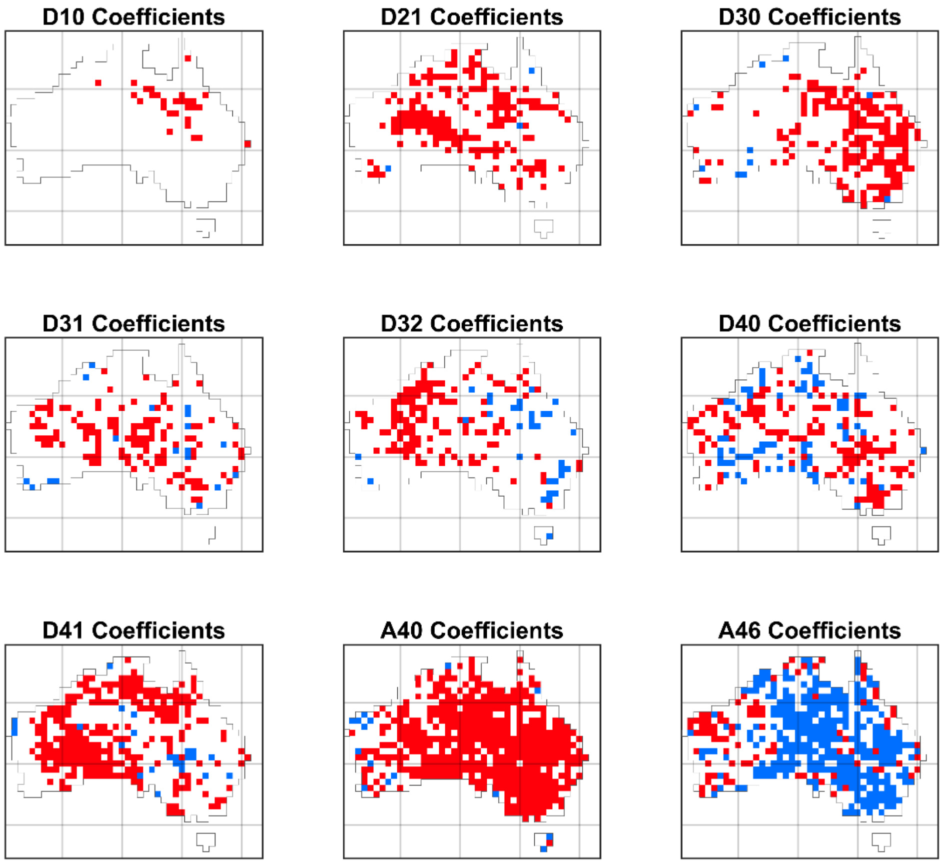


Figure 3A1: Coefficients for all 9 decomposition levels including lags. Red represents a positive coefficient and blue represents a negative coefficient.

4. Dynamic water storage fuels large-scale ecosystem production in water-limited environments

4.1 Abstract

Vegetation dynamics are a core issue of the carbon cycle. When water transpires from a vegetative system, plant growth occurs as a result of photosynthesis, creating a link between the outgoing water flux and productivity. Gross primary productivity is the product of many factors, primarily water availability, along with temperature and solar radiation. The implementation of remote sensing tools such as the Gravity Recovery and Climate experiment (GRACE) and the Moderate-Resolution Imaging Spectroradiometer (MODIS) has made examining global relationships between water dependent processes possible in recent decades. We analyse gross primary productivity as a function of the annual dynamic water storage from GRACE, which represents water moving through a system. Here we show that the dynamic water storage amplitude is a strong driver of biomass production. Globally, highest correlations between gross primary production and annual amplitudes of total water storage are found for water limited ecosystems. The use of total water storage amplitude provides a novel approach for global mapping of the link between vegetation and water dynamics. With predictions of decreased water availability in systems which are already water limited, this relationship could be of great use for future predictions of carbon fluxes and vegetation dynamics.

Key Words

Biomass production, Gross primary productivity, dynamic water storage, GRACE, Water limited ecosystems

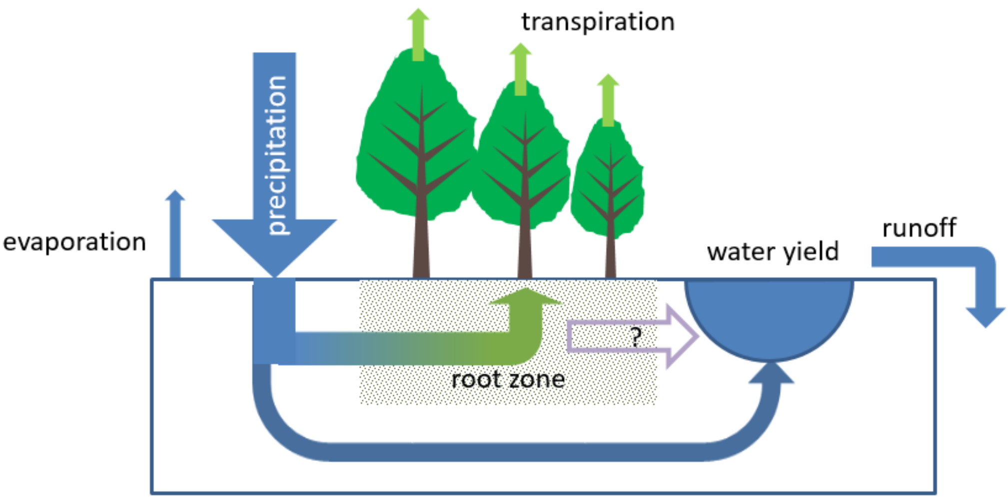
4.2 Introduction

Terrestrial primary production is the largest global carbon sink, and drives important ecosystem functions (Beer et al., 2010). Water limited environments cover approximately 50% of global land mass and are typically considered as water limited because the annual potential evapotranspiration exceeds annual precipitation (Parsons & Abrahams., 1994). In these environments, primary production is susceptible to change because of the dynamic nature of water availability in the critical zone (Newman et al., 2006). Changes in productivity are triggered by climatological, ecological, and anthropogenic influences on the biosphere (Nemani et al., 2003). Our understanding of the controlling environmental variables, driving factors, and ability to measure and predict biomass production is of paramount importance considering the occurring global climate change (Frankenberg et al., 2011).

In recent decades, the implementation of remote sensing products such as the Gravity Recovery and Climate Experiment (GRACE) has made it much easier to examine global water fluxes. Such tools have been widely used for studying hydrological processes and the interaction of water with the biosphere (Wouters et al., 2014). Water availability for terrestrial ecosystems mostly depends on precipitation. Precipitation to the land surface partitions into quick flow component (e.g., runoff or macropore flow quickly recharging groundwater) and slow movement component (e.g., soil moisture). The quick flow components tend to bypass the root zone without contribution to biomass production. It is recently reported that in water limited environments, GRACE Total Water Storage (TWS) appears to be a better predictor of the temporal variability of terrestrial vegetation cover than precipitation (Yang et al., 2014). This finding demonstrates that some precipitation bypasses the biomass-production via runoff and evaporation quicker than can be represented in monthly GRACE data.

Shallow soil moisture has high connectivity with the surface (Good et al. 2015) and may be lost to the atmosphere through evaporation, used by vegetation and lost to the atmosphere as transpiration. In climate zones with distinguished wet and dry seasons, the catchment water storage change in a year, provides an approximation of how much water is used by the ecosystem in the year.

We hypothesize that large scale ecosystem production is controlled by annual dynamic water storage. This concept is shown in Figure 4.1, where hydrological processes bypass biomass production, and other contribute to it. In arid, semi-arid and other water limited environments, soil water availability strongly affects vegetation growth, photosynthesis and survival (Chaves et al., 2002). Depending on the rainfall intensity, precipitation partitions into runoff and infiltration (Dunne et al. 1991) as in Figure 4.1. Runoff and evaporation cannot be used for biomass production but infiltrated water supports transpiration and productivity (Denmead & Shaw., 1962). Depending on the rainfall intensity, precipitation partitions in 'blue' and 'green' water, represented respectively by runoff and infiltration (Dunne et al., 1991). Deep percolating water escapes from the root zone and likely recharges groundwater, which changes at a rate



beyond an annual cycle.

Figure 4.1: The conceptualisation of dynamic water moving through a system. 'Green' water contributes to biomass production. Some components do not affect the water storage amplitude at all such as surface evaporation and runoff.

To test the hypothesis, we examine the relationship between biomass production and annual dynamic water storage as represented by respectively ecosystem annual gross primary production (GPP) and GRACE TWS amplitude (A_{TWS}). GPP is a measure of the amount of CO_2 assimilated by photosynthesis and our ability to estimate it has improved in recent decades (Waring, Landsberg, & Williams, 1998) through the use of remote sensing tools such as the moderate-resolution imaging spectroradiometer (MODIS). We use GRACE A_{TWS} as opposed to simply TWS as this better represents dynamic water storage; water passing through a system. The monthly temporal resolution of GRACE is a rational fit to the residence time of soil moisture, and changes in GPP.

4.3 Data

4.3.1 GRACE data

We use GRACE total water storage (TWS) data from The University of Texas Centre for Space Research (CSR), and NASA's Jet Propulsion Laboratory (JPL) which can be freely downloaded from the GRACE Tellus website (http://grace.csr.nasa.gov/data/get-data/). The suitable post-processing techniques including applying the recommended scaling coefficients were applied (Swenson & Wahr, 2006). The scaling coefficients are in part designed to remove leakage errors and do so significantly (Landerer & Swenson, 2012). Data ranges from March 2003 to December 2014. The gridded data is presented spatially in 100 km by 100 km cells. We selected which cells should be included based on a global shape file. If at least two thirds of the cell was part of a continent they were included, this eliminated some cells which covered only a small coastal area and were mostly ocean.

For the occurrences where a month of data missing in either GRACE data set, the average value from the months either side were calculated and used. This method maintained the seasonal cycle well and was deemed appropriate because of the monthly resolution (Long et al., 2015).

4.3.2 MODIS GPP Data

Monthly GPP data comes from the MODIS product "MOD17A2 gross primary production". The product was freely downloaded from the MODIS website (ftp://ftp.ntsg.umt.edu/pub/MODIS/Mirror/MOD17/Monthly_MOD17A2. The GPP data is produced at a smaller spatial scale (.25 by .25 degrees) than GRACE. They are rescaled to match the GRACE cell size using the resampling tool in ArcGIS. Like the GRACE data, only cells which contain at least two thirds land are used, and missing data are filled by a temporal interpolation of months either side.

4.3.3 Precipitation data

Monthly precipitation data was sourced from the European Centre for Medium-Range Weather Forecasts' (ECMWF) public data set. It was downloaded at the same resolution as GRACE data. The reanalysis data is extracted from the ECMWF model which is partially based on observations. This is a global dataset but only terrestrial precipitation data is used in this study.

4.3.4 Climatic constraint data

Nemani et al., (2003) kindly provided their data of potential climatic constraints to plant growth derived from long-term climate statistics. This data shows the contribution of water, radiation and temperature as a limiting factor of global vegetation growth, where the sum of the 3 contributing factors is 100%. The data are produced at a smaller spatial scale (.5 by .5 degrees) than GRACE and are rescaled to match the GRACE cell size using the resampling tool in ArcGIS. We use only the water constraint component of this data and use it to determine water limited environments. Figure 4.2 shows the distribution of water limitation in increments of 10%. The percentages are relative to the temperature and radiation data, so the higher the value, the more water is a limiting factor in that cell (and the less temperature and radiation are limiting factors).

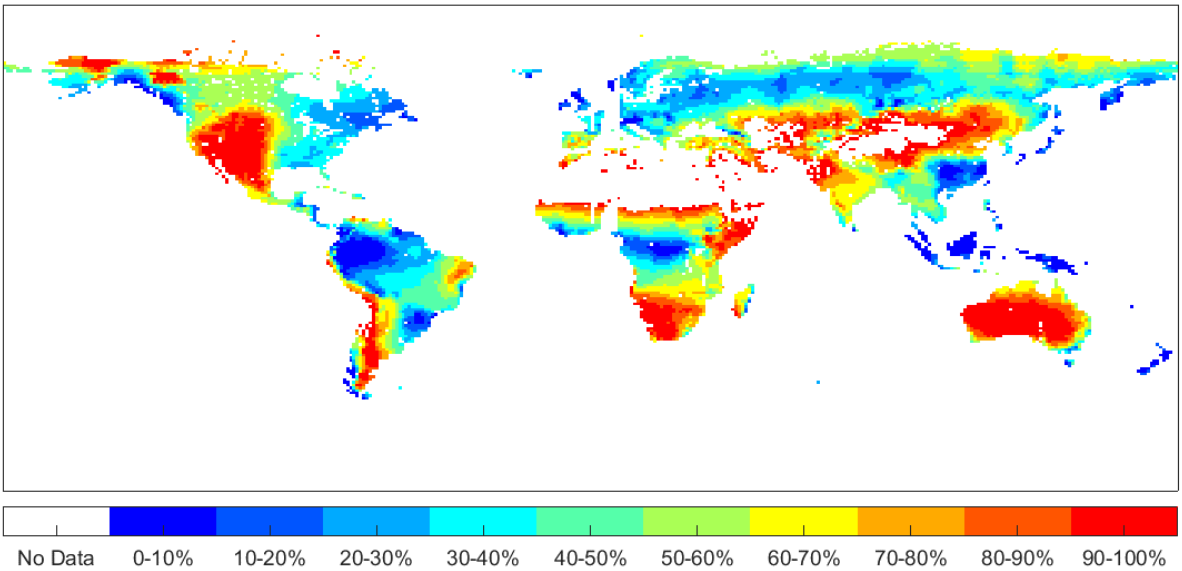


Figure 4.2: The contributing percentage of water constraint on vegetation globally, adapted from Nemani et al., (2003). For this study, areas where the contribution of water constraint to vegetation growth is over 50% are considered water limited.

4.4 Methodology

4.4.1 TWS amplitude calculation

A_{TWS} is calculated in two ways. For an unlagged amplitude, the absolute value of the maximum minus the minimum TWS value in a calendar year is used. For a lagged amplitude, the absolute value of the maximum minus the minimum TWS value in the first six months of a year, and the last six months of the year preceding is used. Where the lagged amplitude is used,

A_{TWS} precedes the GPP/precipitation data i.e. A_{TWS} of 2003/2004 is analysed against GPP/precipitation of 2004 (Figure 4.3).

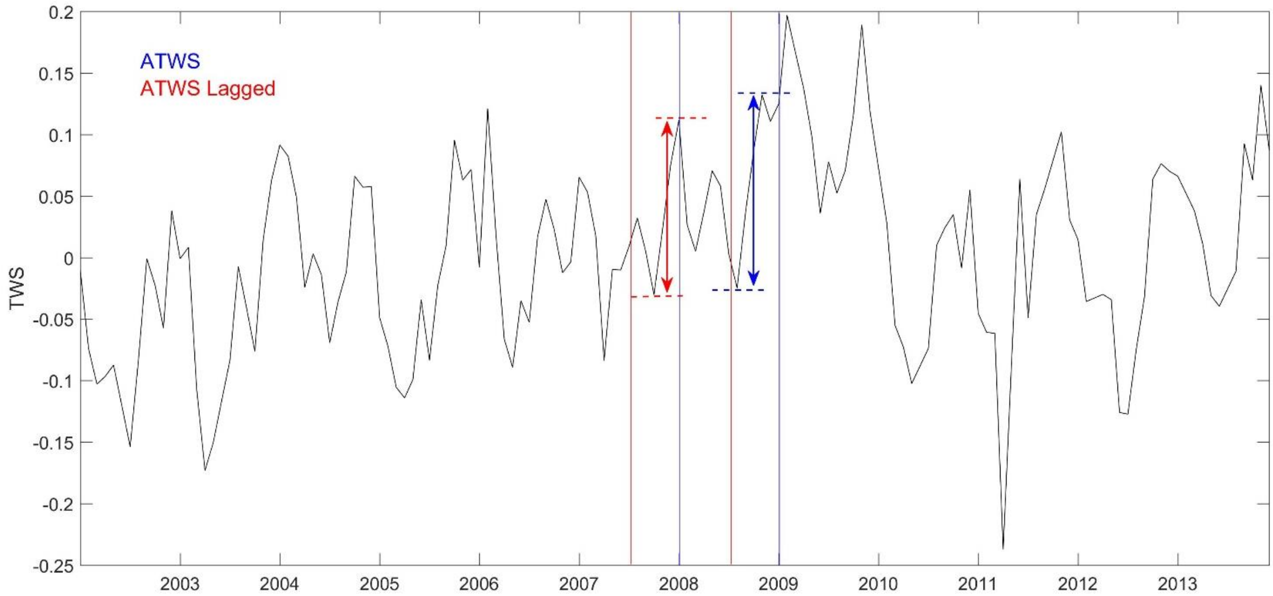


Figure 4.3: An example of how the different amplitudes are calculated. For the time series above, the amplitudes shown would be analysed against GPP data from 2008. The annual amplitude (red) is comprised of the 12 months in 2008. The lagged amplitude (blue) is comprised of the last six months of 2007 and the first six months of 2008 allows for lags between the TWS amplitude and changes in GPP.

4.4.2 Spatial analysis

For a spatial analysis, A_{TWS} ranges with increments of 5 mm are used where the mid-point value of the range e.g. 20mm indicates A_{TWS} data spanning from 17.5 – 22.5mm. The mean of all GPP values within this range is calculated. As a comparison to GPP, precipitation is used instead of GPP, in which case ranges increase in increments of 100mm instead of 5mm. For this analysis A_{TWS} are calculated only using data from the same calendar year, not part of the preceding year. For both precipitation and GPP, five tests are done for regions of different water limitation ranges. These include areas where water stress contributes to limiting vegetation growth by 50-60%, 60-70%, 70-80%, 80-90% and 90-100%. R^2 values are calculated for each water limitation range.

4.4.3 Temporal Analysis

For a temporal analysis all data from each cell considered to be water limited is analysed separately using the span of available data (2003-2014). Pearson's coefficient (*r*) is used to evaluate the strength of the relationship between A_{TWS} and GPP. The same analysis is carried out using precipitation instead of GPP. For this analysis, both the lagged and unlagged A_{TWS} data are used and the highest *r* value from the two approaches is shown in the results.

4.5 Results

Figure 4.4 shows the results of the spatial analysis between precipitation and GPP in areas of increasing water limitation (Figure 4.4 (a)-(e), 50-60% to 90-100% respectively).

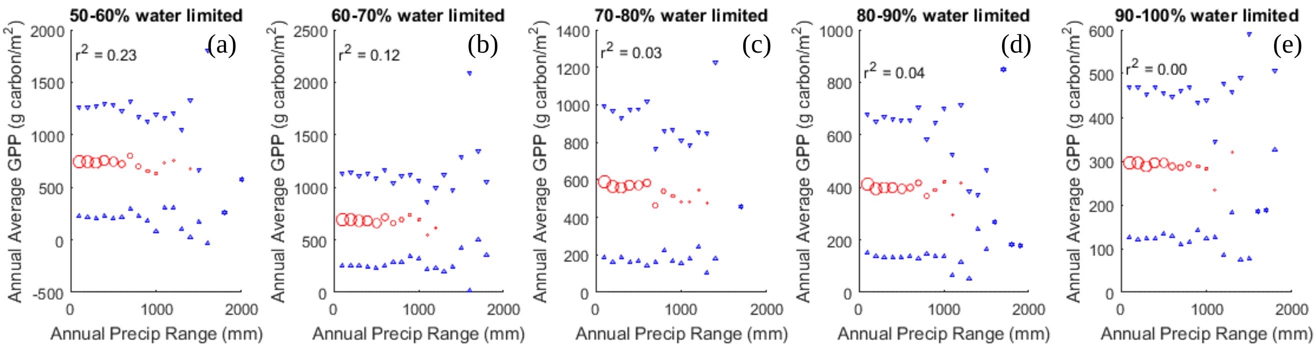
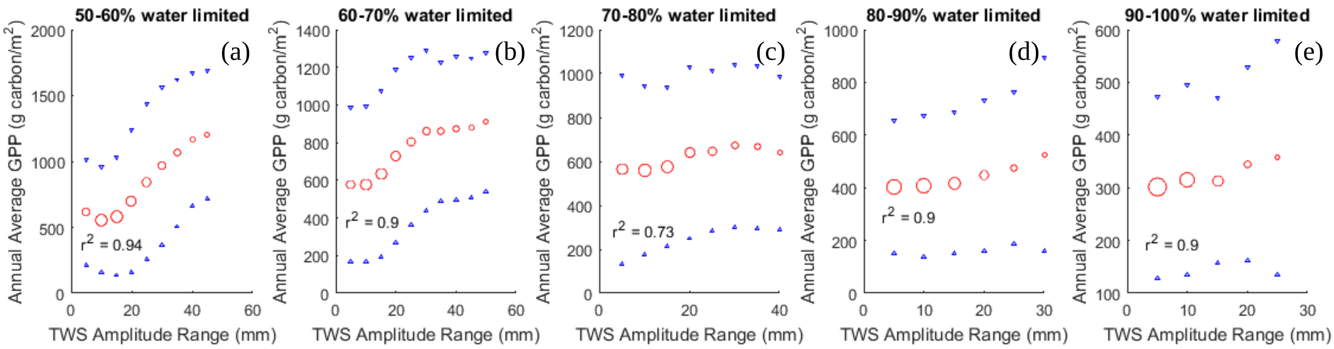


Figure 4.4: The mean GPP value for different precipitation ranges across different increments of vegetation water dependence. Red markers show the relationship, with their size being relative to the number of cells in each range. Blue markers denote +/- one standard deviation.

The relationships in figure 4.4 for the different increments of water as a limiting factor show very poor correlations. The highest r^2 value (0.23) is in the 51-60% range though even that result is not significant. These results are as expected and likely due to the fact that not all precipitation is used by vegetation (Chen et al., 2014) and some is lost through runoff, evaporation etc. Figure 4.5 shows the results of the spatial analysis between A_{TWS} and GPP in water areas of increasing water limitation (Figure 4.5 (a)-(e), 50-60% to 90-100% respectively)

Not only does this show that the relationship between A_{TWS} and GPP is not simply an artefact of precipitation, it also further supports that in water limited environments biomass production is



controlled by dynamic water storage.

Figure 4.5: The mean GPP value for different A_{TWS} ranges across different increments of vegetation water dependence. Red markers show the relationship, with their size being relative to the number of cells in each range. Blue markers denote +/- one standard deviation.

For the given data, GPP is highly correlated to A_{TWS} in water limited environments. R^2 values range from 0.73 – 0.94, however there is no clear increasing or decreasing pattern through the different increments of water limitation. As the water limitation becomes stronger, the A_{TWS} range decreases, as does the overall mean GPP value. A higher proportion of cells fall into the lower A_{TWS} ranges as the increment of water limitation increases, with a more even distribution in the lower increments. Furthermore, the three lower increments of water limitation show small negative correlations between GPP and A_{TWS} for the first two points. While still strong, areas that are 71% - 80% limited by water show the worst relative correlation which is poor compared to the others. The last two points show a negative correlation though the overall trend is positive.

The temporal relationship between precipitation and GPP for each water limited cell globally is shown in figure 4.6. The strength of the relationship is measured by Pearsons Coefficient (r).

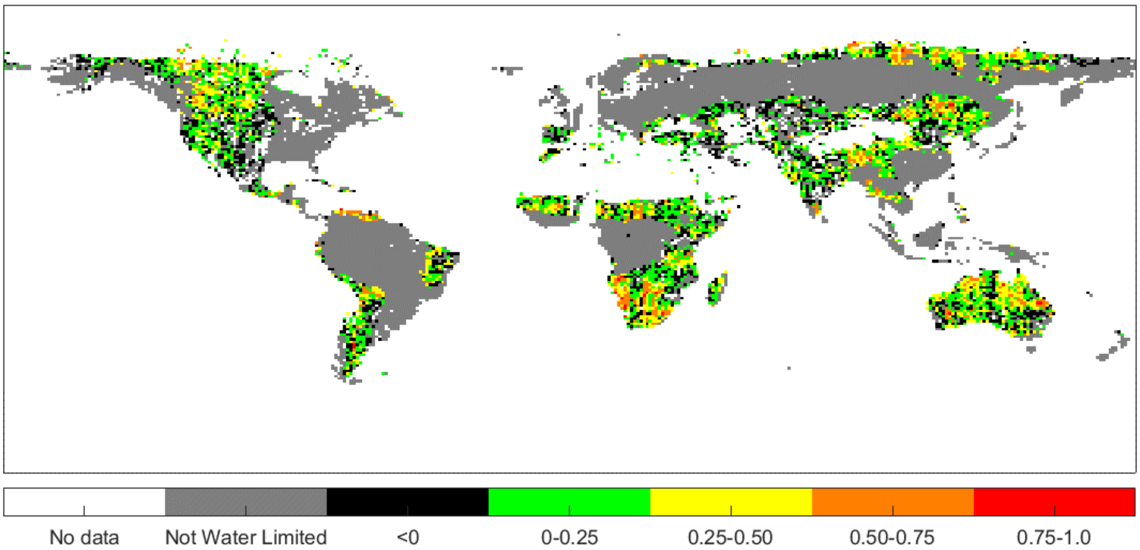


Figure 4.6: The relationship between GPP and precipitation for water limited environments globally, shown by Pearson's coefficient (*r*). In water limited environments the relationship is poor.

Only 54.6% of cells show a positive relationship between precipitation and GPP. Where positive *r* values exist, few exceed .50. There does not appear to be any spatial coherence among similar *r* values, and negative values are scattered somewhat randomly throughout. The relationship between GPP and precipitation does not seem to be similar to different spatial patterns of aridity, climate, land use etc. The temporal relationship between A_{TWS} and GPP for each water limited cell globally is stronger overall (figure 4.7).

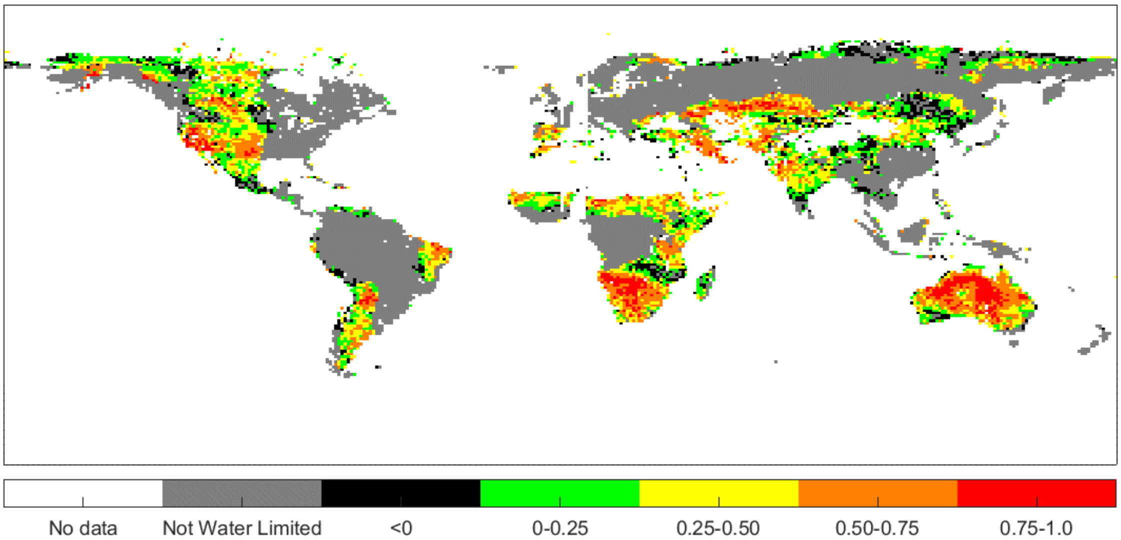


Figure 4.7: The relationship between GPP and A_{TWS} for water limited environments globally, shown by Pearson's coefficient (*r*). In water limited environments the relationship is generally strong and performs better than GPP vs precipitation.

Globally, 79.5% of water limited areas show a positive relationship between GPP and A_{TWS}. This is significantly higher than the GPP-precipitation relationships shown in figure 4.6. Generally, there is spatial coherence of areas with relationships of similar strength, whether it is a positive or negative relationship. However, some areas show random positives amongst negatives or vice versa. The strongest and most spatially coherent relationships are seen in Australia, South Africa, western U.S.A and parts of Europe. There is a pattern of higher correlations existing further inland and lower correlations tending towards the coast. Australia is a very good example of this. Data from a large part of Northern Africa is missing from the MODIS data set, though being a highly water limited, arid region similar to central Australia (Yang et al., 2016), presumably this area would show a very strong correlation, likely further improving the overall relationship.

Based on Pearson's coefficient, the strongest relationship between A_{TWS} and GPP was found using the lagged amplitude method in 52.9% of cells, while 47.1% of cells had a higher correlation using an amplitude calculated from values in the same calendar year (Figure 4.8).

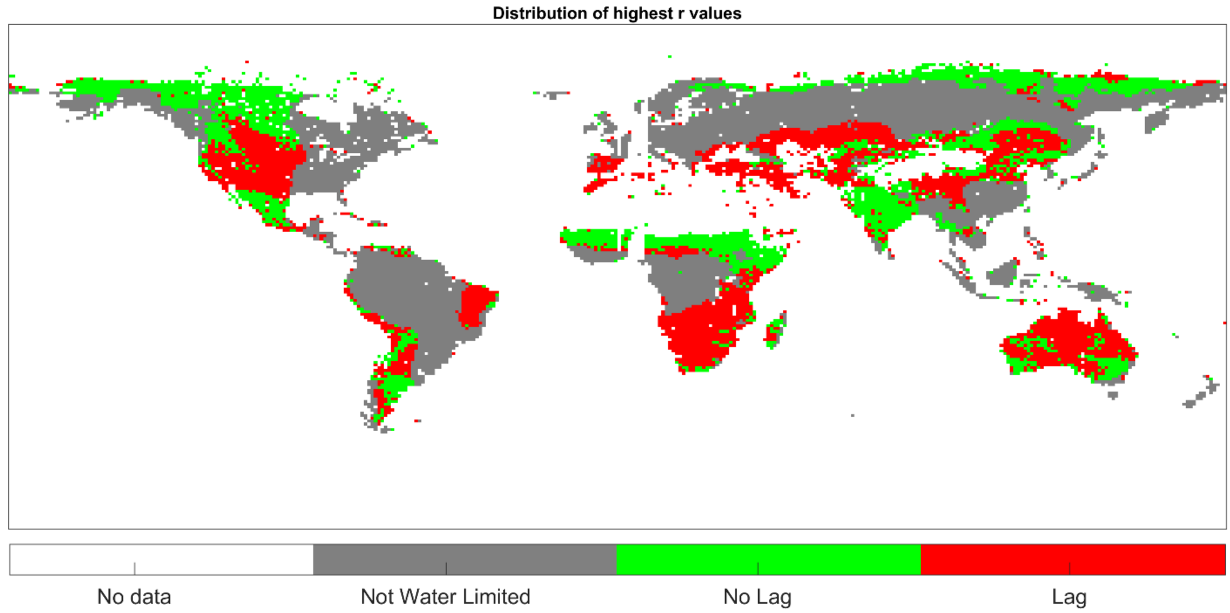


Figure 4.8: The distribution of the highest performing *r* value based on the method of calculating amplitude. There is clear spatial coherence between the two methods, with a slightly larger area showing a lag between changes in A_{TWS} and GPP.

Although the almost equal amount of cells that favour each amplitude method in figure 4.8 is what would be expected from chance alone, the clear spatial distribution of two methods suggests that this is not the case. The lagged method shows a better relationship in areas which have an overall higher *r* value in Figure 4.7. These include Australia, South Africa, Europe and parts of North and South America. This suggests that there is a lag of up to six months between water moving through these systems and significant biomass production. Without a lag in the amplitude, parts of India, Africa, Australia and North and South America show a higher relationship. In particular, the most northerly sections of land, comprised of Russia and North America show almost exclusively the highest correlation coming from the un-lagged amplitude. However, these areas are often snow-covered and have little vegetation, potentially skewing the results. In contrast to areas favoured by the lagged amplitude, these areas are generally humid or subhumid (Yang et al., 2016). Again, as the region of missing in Africa that closely matches that of central Australia in terms of aridity, climate and vegetation cover, presumably this area would also show a better relationship using the lagged amplitude data.

4.6 Discussion

4.6.1 Significance of relationship

The results from the spatial analysis in this study demonstrate that there is a strong relationship between A_{TWS} and GPP, suggesting that biomass production as represented by GPP is driven strongly by dynamic water storage at a pace captured by GRACE. Importantly, a large discrepancy appears between results using precipitation and results using A_{TWS} which demonstrates that the time series of A_{TWS} are not simply precipitation driven. In figure 4.5, the strength of the relationship does not necessarily improve as water becomes more of a limiting factor of vegetation production; on average the relationship slightly decreases. This could be attributed to the sample size and spread of data. The higher the water limitation, the fewer cells are included in the analysis. Furthermore, the distribution of these cells becomes less even as the water limitation increases, skewing the slope to the lower amplitude ranges. There is nothing conclusively showing that dynamic water storage drives biomass production differently depending on how water limited an area is, just that this is the case in general in water limited environments. The results from 51-60%, 61-70% and 71-80% water limited areas show a negative correlation in the first two points. This suggests that in areas of less dynamic water storage, biomass production is not as sensitive due to precipitation having less seasonality.

The results from the temporal analysis in this study demonstrate that there is a strong relationship between A_{TWS} and GPP that varies spatially. Similar results show clear spatial coherence, validating the strength of the relationships and study. The results from the temporal analysis further demonstrate a far superior relationship between GPP and A_{TWS} than GPP and precipitation, demonstrating that neither biomass production nor A_{TWS} are simply precipitation driven.

Generally, areas which show a stronger relationship between lagged A_{TWS} and GPP are those with the highest percentage of water as a limiting factor, roughly above 80%. This pattern is relatively consistent globally and such areas are prone to drought or prolonged periods of aridity.

The distribution of areas in which lagged or un-lagged data shows the strongest relationship is loosely correlated with different climate zones. This in turn relates to other clarifications such as land cover type and aridity index which have very similar spatial distributions globally. Zones of land cover type, climate etc. are generally classified based on long term averages. Because we only use 12 years of data, it is likely that some patterns within these 12 years are different to long term averages, causing the spatial distribution of the best correlating amplitude to show deviations from different climate zones. An example is Australia's millennium drought, which spanned for over half of the study period, in which time, hydrological and vegetative behaviours were much different to long term averages.

4.6.2 The advantage of using amplitude

Gridded GRACE TWS data is presented as an equivalent water thickness in cm with respect to each cells own long term mean (Wahr et al. 1998). As each cell is referenced to itself, the data is generally directly comparable spatially. However, using the amplitude of each cell allows for the cells to be compared directly spatially as the long term mean is neglected and only the total flux in and out of a cell is considered.

4.6.3 Potential for use as an indicator of GPP

This study further demonstrates the potential use of GRACE. In a time of globally changing hydroclimatic conditions, predictions of GPP are important for understanding potential future changes in the carbon cycle and vegetation dynamics (Huxman., 2004). This further highlights implications of land use change which can highly influence hydrological conditions (Li et al., 2009). Numerous models have been created to estimate GPP in different parts of the world, over different periods of time (Ruimy et al., 1996) (Williams et al., 1997) (Sims et al., 2008). One independent study compared estimates from 26 GPP models to estimates from 39 eddy covariance flux tower sites and found that none of the models matched estimated GPP within the range of uncertainty of observed fluxes (Schaefer et al., 2012). Aside from seemingly poor performance, many models require considerable input from ground based meteorological measurements (Sims et al., 2008) which can be hard to access or temporally and spatially sparse (Chen et al., 2013). An alternative to models is using the strong relationship we have found, as abundant relative total water storage data exists. Because water highly influences GPP and water storage forecasting tools are becoming increasingly available (Todini., 1988), the usage of total water storage amplitude fits well as a potential indicator of GPP.

4.7 Conclusion

Our findings show that overall there is a very strong correlation between A_{TWS} and GPP. This demonstrates that biomass production is dependent on dynamic water storage in water limited environments. The strength of this relationship varies spatially, however stronger correlations are generally spatially coherent, making it easy to identify where dynamic water storage is a strong driver of biomass production. Spatial differences in how GPP correlates to lagged or un-lagged A_{TWS} does not demonstrate how GPP responds to water storage dynamics in different climate zones, likely due to the temporal resolution of the study. The relationship is clearly not an artefact of precipitation. Furthermore it outperforms the relationship between precipitation and GPP across water limited environments globally. Coupled with hydrological forecasts and models, this understanding of dynamic water storage as a driver of biomass production could help generate significant improvements in future predictions of the carbon cycle as well as vegetation dynamics. This is especially useful for highly water limited areas which are at risk of extreme hydrological events such as drought and or changes in ecosystem behaviour and GPP.

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5. Conclusions

5.1 Summary of findings

The aim of the studies in this thesis was to improve our understanding of relationships between terrestrial water and vegetation on a continental and global scale while extending the potential application of GRACE by using it in innovative and previously unused ways. The three chapters in this PhD thesis examined terrestrial water-vegetation interactions and make scientific advances towards our understanding of such processes. Each study used GRACE as the primary data source. Overall findings show that more than just total water storage data can be extracted from GRACE when filters such as a wavelet are applied. This is useful for partitioning GRACE into different vertical moisture storage components and revealing the moisture dependence of vegetation in different land use types. It is also shown that biomass production is driven by dynamic water storage in water limited ecosystems, and the annual amplitude of GRACE represents this dynamic water storage well.

The key findings from each of the 3 individual studies are as follows:

(i) A new method for estimating various water storage components across Australia using decomposed GRACE data, with the AWRA model as a reference was developed. A stepwise regression was successful in determining which decomposed TWS frequencies should be used in the estimation of different storage components for each cell. An analysis of the decomposed GRACE data compared to raw GRACE data showed that decomposing the data improved its correlation to the AWRA model, increasing R^2 values and decreasing the RMSE. The estimations for shallow and deep water stores showed a clear improvement on raw GRACE data when compared to the AWRA model.

(ii) Combinations of decomposed GRACE TWS* data show an improved relationship with NDVI* over raw GRACE TWS* alone. Varying decomposed frequencies show spatial coherence for parts of Australia, sometimes independently and sometimes overlapping other decomposed frequencies. Generally, NDVI is influenced by low frequency changes in water storage, however there are some areas which are also sensitive to high frequency changes. NDVI is susceptible to a memory effect which depends on previous TWS conditions with a 6 months delay generally. The total influence of NDVI changes is made up of storage changes over different time periods. These vary depending on the land use type and the results are aligned with our physical understanding.

(iii) On average globally there is a very strong relationship between the annual GRACE TWS amplitude and gross primary production. This demonstrates that biomass production is dependent on dynamic water storage. The strength of this relationship varies spatially, however stronger results are generally spatially coherent, making it easy to identify where dynamic water storage is a strong driver of biomass production. Spatial differences in how gross primary production results to lagged/un-lagged GRACE TWS amplitude demonstrates how gross primary production responds to water storage dynamics in different climatic zones. The relationship is clearly not an artefact of precipitation. Furthermore it outperforms the relationship between precipitation and gross primary production across water limited environments globally.

The conclusions from the research presented in this thesis demonstrate significant contributions to studies of ecohydrology, as well as the potential use of GRACE, and implications to the carbon budget.

5.2 Future work

In a time of global climate and land use change, it has never been so important to understand how water resources and vegetation interact. Luckily, the implementation of remote sensing tools such as those used throughout this thesis mean that our ability to study such changes over continental or global scales has never been so strong. Several suggestions for future work that expands on the research in this thesis are given below.

(i) Wavelet decomposition to extract signals from GRACE has proven to be a relevant methodology. This method could be further extended to make it even more useful, depending on the application. For the study in this thesis, the AWRA model is used as a reference. Only subsurface moisture stores are considered. There is potential for other models or observations to be used such that GRACE is partitioned into further components such as vegetation water stores and different surface and subsurface moisture stores.

(ii) As the GRACE mission continues, longer data sets will become available and it will become more feasible to decompose the data beyond 4 levels, resulting in more precise outcomes. Alternative wavelet functions of methods of decomposition could also be explored which may suit different data types or geographical environments better.

(iii) Superconducting gravimeters can create estimations of subsurface water storage similar to GRACE, but at a point scale (Cruetzfeldt et al., 2012). Further research could be conducted to see how the wavelet decomposition method could potentially be applied to such measurements. If succesful this could be an extremely useful tool and more practical than GRACE at field scales. Based on the test conducted with soil moisture in chapter 2, this should give promising results at such a scale.

(iv) Chapter three of this thesis used the wavelet decomposition method to reveal the moisture dependence of vegetation at different temporal frequencies. Similar studies could be carried out with other variables which are water dependent instead of NDVI. Examples include variables such as land surface temperature, soil carbon content and respiration, etc.

(v) Even without decomposition, GRACE can be used to represent more than just total water storage, such as dynamic water storage – water passing through a system. There is potential for further uses of GRACE to represent different hydrological processes. Finding and understanding such uses of GRACE could further assist our understanding of hydrological processes on a continental/global scale.

It is an important (and exciting) time to work with products such as GRACE, which clearly hold more information than meets the eye. Future development of innovative ways to use GRACE to its full potential open up numerous opportunities to develop our understanding of interactions between hydrology and the biosphere, working towards a healthier and more sustainable planet.

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