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Satellite-Based Data-Driven Modelling of Inland Green-Blue Ecosystems

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NOVA Information Management School
Instituto Superior de Estatística e Gestão de Informação

Universidade Nova de Lisboa

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SATELLITE-BASED DATA-DRIVEN MODELLING OF INLAND GREEN- BLUE ECOSYSTEMS

by

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Doctoral Thesis presented as a partial requirement for obtaining the PhD in Information
Management

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July 2024

STATEMENT OF INTEGRITY

I hereby declare having conducted this academic work with integrity. I confirm that I have not used plagiarism or any form of undue use of information or falsification of results along the process leading to its elaboration. I further declare that I have fully acknowledged the Rules of Conduct and Code of Honor from the NOVA Information Management School.

Bruna Almeida

Lisboa, July 01, 2024

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ABSTRACT

Technological advances in Satellite Earth Observation (SEO), decision systems and geoinformation are revolutionizing the assessment of natural assets. The evolving integration of satellite-based Machine Learning (ML) techniques into Green-Blue Ecosystems (GBE) modelling demands a deeper understanding of applications across scales, and the identification of avenues for future research. To study the relationship between aquatic and terrestrial ecosystems, an assessment framework with methods, concepts, and models was developed. It includes a set of tools with reference data and guidelines, based on reviewing well-established and innovative techniques reported worldwide. The research is divided into three main phases: Conceptualization and Design (Stage 1), Proof of Concept (Stage 2), and Development and Implementation (Stage 3). The main output of Stage 1 is a systematic literature review and meta-analysis focused on studies that have developed ML models to estimate Ecosystem Services indicators based on high-resolution and open-access satellite data. Stage 2 demonstrates the feasibility, robustness, and replicability of research. The main outputs of this stage are modelling different spatial and temporal scales, and testing data and methods, providing guidelines to basis the development and implementation of research at the country level. At the development and implementation stage, the main outputs are the GBE capacity provisioning assessment at the national level and the spatial and temporal multiscale mapping of carbon storage and sequestration by forest ecosystems in Portugal's mainland. This dissertation contributes to advancing the knowledge of GBE, unveiling the potential of satellite-based data-driven models, understanding ecosystem dynamics, drivers of changes, modelling conceptualization, development, and implementation. Findings link the current knowledge to integrated models that include key aspects of GBE drawing on science-technology-innovation, presenting guidelines for the assessment of GBE from SEO, and filling the gap with advanced knowledge related to consistent GBE information across multiple scales.

KEYWORDS

Remote Sensing; Machine Learning; Geographic Information Systems; Aquatic Ecosystems, Terrestrial Ecosystems; Natural Capital

Sustainable Development Goals (SGD):



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LIST OF ABBREVIATIONS AND ACRONYMS

CSS	Carbon Storage and Sequestration
DL	Deep Learning
EA	Ecosystem Accounting
ES	Ecosystem Services
ESi	Ecosystem Services indicators
ESDA	Exploratory Spatial Data Analysis
FCD	Forest Cover Density
FWPI	Freshwater & Wetness Probability Index
GBE	Green-Blue Ecosystems
GIS	Geographic Information Systems
LULC	Land use and land cover
ML	Machine Learning
NUTS	Nomenclature of territorial units for statistics
RE	Reverse Engineering
RS	Remote Sensing
SDG	Sustainable Development Goals
SEEA-EA	System of Environmental-Economic Accounting-Ecosystem Accounting
SEO	Satellite Earth Observation
TCD	Tree Cover Density
UN	United Nations
WWPI	Water & Wetness Probability Index

1. INTRODUCTION

1.1. BACKGROUND

The importance of Green-Blue Ecosystems (GBE) namely the role played in the context of natural capital and sustainable development goals, justifies the interest of the author on these topics. Of the foundations considered as a reference for the research, some of the initiatives aiming to establish policies for the conservation of natural resources stand out, such as the sustainable development goals proposed by the United Nations for the 2030 Agenda.

This research directly supports five of the 17 goals (3, 6, 11, 13 and 15) and can be used as a benchmark for better understanding the drivers of changes in GBE, finding alternative ways of achieving sustainable well-being, diversity, resilience, and to evaluate contributions from conservation projects, payment schemes, and new governance approaches at different scales.

GBE encompass both terrestrial and aquatic ecosystems, including forests, croplands, wetlands, rivers, and lakes. The intricate interplay between aquatic and terrestrial ecosystems is often observed in riparian areas, where rivers are surrounded by vegetation, and in locations where groundwater interacts with water bodies (Bertrand et al., 2012; Eamus & Froend, 2006a). This relationship is influenced by various biophysical parameters, such as climate, hydrology, topography, and human activities (X. Yang et al., 2021a). Drivers such as groundwater over-abstraction, land-use conversion, and climate change contribute to significant changes in GBE (Mpakairi et al., 2022a).

GBE relies heavily on climatic variables like precipitation, evapotranspiration, solar radiation, and wind, as well as factors involved in carbon and water cycles (Gwal et al., 2020). Terrain conditions and the presence of groundwater, influencing phreatophyte vegetation, play crucial roles in determining GBE health and behaviour (Dwire et al., 2018). Seasonality, particularly during dry periods marked by low rainfall, high temperatures, and increased evapotranspiration, significantly impacts these ecosystems, leading to the drying out of seasonal wetlands, reduction in vegetation heterogeneity, crop production, and water yield (Kundu et al., 2022).

On a global scale, research has demonstrated the significant influence of Land use and land cover (LULC) changes on the delivery of Ecosystem Services (ES) (Rijal et al., 2021). Accurate and timely information on spatial and temporal changes in LULC is vital for understanding the dynamic relationship between the environment and society (Mengist et al., 2021). The value of ES is positively linked to vegetation and water extent but negatively correlated with bare land area (X. Wang et al., 2021).

Forests, cultivated lands, rivers, and lakes emerge as key biomes for ES provisioning and regulation (Mugiraneza et al., 2019). The condition of habitats directly impacts service availability (McVittie & Hussain, 2013). Mapping biodiversity, species distribution, and landscape characteristics allows for the measurement of ecosystem capacity provision, its utilization, and its value (Grêt-Regamey et al., 2014). However, as competition for land use intensifies due to urban sprawl, agricultural practices, and climate change, the management of natural resources faces challenges, leading to ongoing biodiversity losses (Skidmore et al., 2021).

ES Indicators (ESi) such as carbon storage, timber supply, food productivity, water yield, and nutrient cycling offer insights into ecosystem conditions, aiding in their assessment (Gwal et al., 2020). Forests, acting as crucial sink sources of atmospheric carbon, require monitoring of spatiotemporal vegetation dynamics to understand changes in biomass resulting from various factors (Jiang et al., 2022).

The intricate relationships between surface waters, groundwaters, and anthropogenic pressures impact aquatic ecosystems that provide essential services, including habitat provision, nutrient uptake and aesthetic values (Haines-Young et al., 2012). Monitoring hydrological services becomes imperative to comprehend their status, functioning, and responses to pressures (Pipia et al., 2021). Assessing crop yields is crucial for effective agricultural management, influencing ES such as food production, biodiversity, climate regulation, pollination, and water provision (Morell-Monzó et al., 2020).

In the context of climate change, Portugal is recognized as a hotspot among the most vulnerable European countries (Marques et al., 2019). Recent studies have shown evidence of climatic changes, such as the long periods of drought recorded in 1990 and 2012 (Almeida & Cabral, 2021). Decreased precipitation, or its greater frequency and intensity in the winter, or large variations over short periods, is leading to substantial decreases in the water yield (Chrysafis et al., 2020). The crop fields are also affected and depend more on irrigation, as well as water quality, which is increasingly compromised, either directly by the increase in salinity caused by rising temperatures, marine intrusion or anthropogenic pollution (Q. Wang et al., 2023).

The status and conditions of GBE depend on climatic conditions which explains the decreased values observed in the natural capital in the last 30 years. Deforestation, environmental pollution, and the overexploitation of resources, together with the natural cycles of the Earth are scaling up the consequences of climate changes in the delivery of values from nature. Technological advances in the domain of Remote Sensing (RS), computational resources and decision systems are revolutionizing the assessment of natural assets.

Integration of Satellite Earth Observation (SEO) data with data-driven modelling is one of the most promising approaches to developing timely and accurate environmental monitoring systems (Reddy, 2021). Unlocking the potential of SEO data & technologies to assess inland GBE supports the implementation of integrated management of natural resources, prioritizes actions to combat climate change and its impacts, and halts and reverses land degradation and biodiversity loss.

Therefore, the lack of guidelines for implementing satellite-based environmental models is a challenge for those who support decision-making with geospatial information (Jullian et al., 2021). RS applications suggest a standardized approach to monitoring ecosystem changes, recording the services they provide, and linking this information to economic and other human activities (Czúcz et al., 2021). SEO data and technologies support the monitoring of ES, and geographic information systems (GIS) provide tools to build spatially explicit models to assess them. In this perspective, this dissertation aims to contribute to advancing the knowledge of GBE developing satellite-based data-driven models to assess aquatic and terrestrial ecosystems at multiscale.

The research combines SEO data and technologies with data-driven approaches to assess natural resources stocks, land use and ES through modelling GBE (Figure 1.1). SEO data allow the derivation of ecologically meaningful information and represent a valuable tool for continuous, large-scale monitoring applications (Holzwarth et al., 2020). It supports building long-term observational records

of environmental changes and estimates biophysical indicators of vegetation and surface conditions at both temporal and spatial scales (Khwarahm, 2021). The data-driven modelling involves collecting and analyzing data and identifying patterns, trends and correlations through statistical methods, data visualization and descriptive analytics (Lee et al., 2023). The opportunities associated with these technological innovations include the potential for gathering, processing, analyzing and visualizing a wide variety of data, and integrating socio-economic and environmental information (Fleming et al., 2022). Advancements in geospatial techniques, such as satellite imagery, geospatial mapping, drones, and sensors, are viewed as highly promising to improve decision-making on both individual and cross-sectoral levels facilitating the deployment of Ecosystem Accounting (EA) and the possible alternative uses for this land (Farrell et al., 2021).

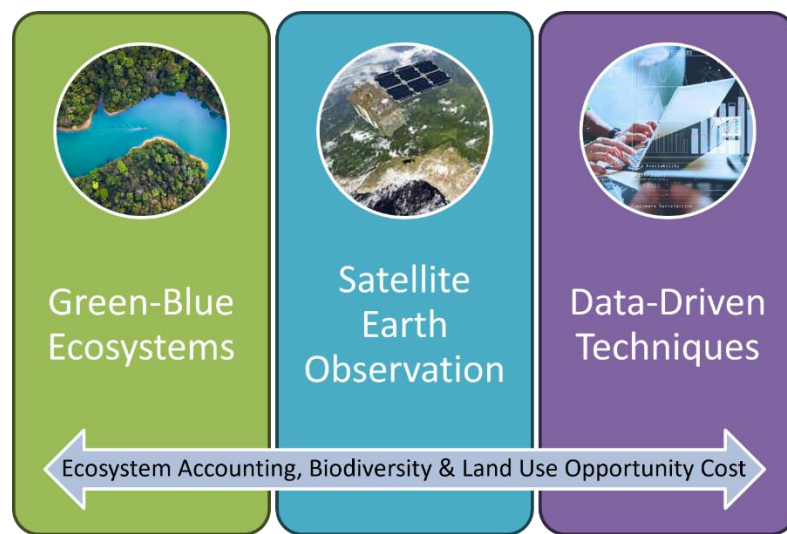


Figure 1.1 - Research concepts.

Ecosystem Accounting offers a framework for quantifying and valuing the interactions between ecosystems, society, and the economy (Edens et al., 2022a). These accounts assess the extent, condition, and services of ecosystems, offering a standardised way to measure biodiversity and natural capital and address ecological degradation (King et al., 2024). Moreover, they aid in comprehending the risks and dependencies of economic activities on the environment and monitoring progress toward sustainable development (Alarcon Blazquez et al., 2023). Within the realm of natural capital accounting, ecosystems are considered assets that provide goods and services to society (Bordt, 2018; Hein et al., 2020). These analyses contribute to a holistic comprehension of the complex interconnections among human activities, land use, and the dynamics of ES.

1.2. OBJECTIVES, RESEARCH STRUCTURE AND EXPECTED OUTCOMES

Despite existing studies focusing on modelling the assessment of GBE through SEO and ML, there is a gap in understanding the relationship between those concepts, modelling conceptualization, development and implementation. To study the relationship between aquatic and terrestrial ecosystems, an assessment framework with methods, concepts, and models is developed. It includes a set of tools with reference data and guidelines, based on reviewing established and innovative techniques reported worldwide. The central role of this research is to produce guidelines for the

assessment of GBE from SEO and fill the gap with advanced knowledge related to consistent GBE information at the national scale. The specific aims are to: 1. Assess the potential of satellite data and technologies to map GBE; 2. To study the relationship between aquatic and terrestrial ecosystems; 3. Implement satellite-based data-driven models to assess the status of GBE for continental Portugal; 4. Discuss and analyse the major aspects of integrated GBE assessment, and the impacts of LULC and climate changes; 5. Build a conceptual framework for assessing GBE, and provide guidelines and reference data that can be used for modelling GBE at multiscale.

The present document includes five chapters: Introduction (Chapter 1), Research Conceptualization and Design (Chapter 2), Proof of Concept (Chapters 3 and 4), Research Development and Implementation (Chapter 5 and 6), and Conclusion (Chapter 7). The research is conducted following the diagram flux (Figure 1.2) divided into three main phases: Conceptualization and Design (Stage 1), Proof of Concept (Stage 2), and Development and Implementation (Stage 3).

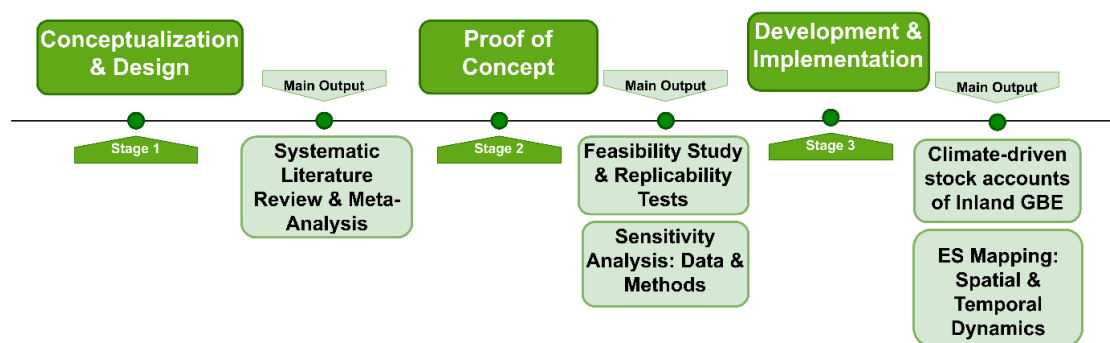


Figure 1.2 - Research structure.

Stage 1 (Chapter 2) starts exploring the research concepts following the building blocks of theory development proposed by (Whetten, 1989), including the essential elements for a phenomena explanation: what, how, why, when, who and where. The main output of Stage 1 is a systematic literature review and meta-analysis focused on studies that have developed ML models to estimate ES based on high-resolution and open-access satellite data. The chapter includes the synthesis of key methodologies, a comprehensive overview of the current state of research in this domain, and answers the following research questions: i. Which SEO data are used for modelling ESi? ii. Which ESi are assessed using SEO and ML techniques? iii. Which ML models are implemented? iv. What is the relationship between ML tasks and ESi? v. Is there a rule for model development within ESi? Since a major use of meta-analyses is to provide baselines for future studies, we use the results to design the research and guide the research development and implementation. Figure 1.3 depicts the stage 1 conceptual model.

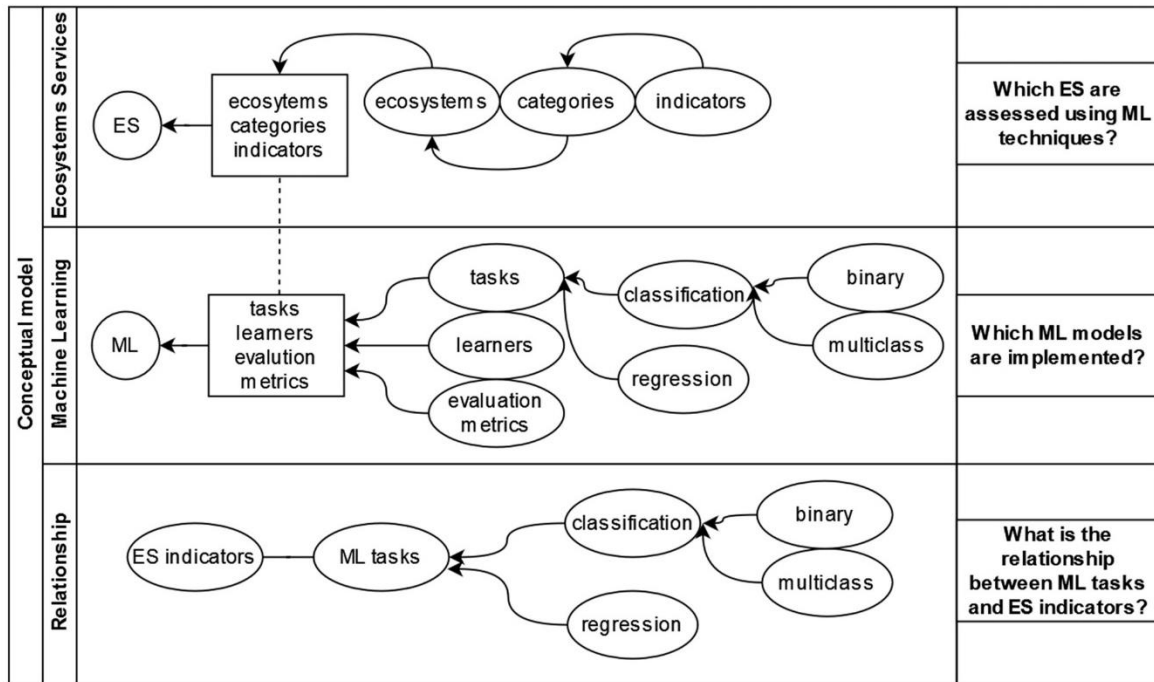


Figure 1.3 - Stage 1: Conceptual Model.

Stage 2 regards demonstrating the feasibility, robustness, and replicability of research. A feasibility study methodically assesses essential aspects of the research, such as examining the viability of spatial and temporal data, while sensitivity analyses evaluate the confidence of data and methods, and reverse engineering techniques guide the replicability and reproducibility of methodologies. The main outputs of this stage are modelling different spatial and temporal scales, and testing data and methods, providing guidelines to basis the development and implementation of research at the country level. This stage includes two published scientific productions presented in chapters 3 and 4. The study depicted in Chapter 3 has the goal of applying sensitivity analyses to test and find the best predictors for modelling freshwater ecosystems. It provides a framework of global geospatial data, and application baselines to support estimating Water Water Productivity Index (WWPI) in different spatial and temporal scales. Chapter 4 presents a study combining techniques to take advantage of different methods by developing a hybrid modelling approach to map GBE and estimate their relationship considering seasonality. This study proposes a two-step modelling strategy that helps to manage and analyze effectively large geospatial datasets while enhancing overall efficiency in GBE mapping workflows.

At the development and implementation stage, the main outputs are the GBE capacity provisioning assessment at the national level and the spatial and temporal multiscale mapping of climate regulation services. Chapter 5 proposes a methodology that relies on Reverse Engineering to reproduce Tree Cover Density (TCD) and WWPI taking into consideration climatic and topographic factors to be further used as proxies to evaluate the capacity of GBE to provide ES. Chapter 6 presents the research outcomes of modelling the characterization of forest ecosystems in Portugal's mainland, assessing two of five SDG 15.2.1 sub-indicators: 1) the annual net change rate of forest area between 2018 and 2022, and 2) the estimation of AGB stored in the forest in the studied years. Chapter 7 summarises research findings, the contribution remarks of each research stage, and points out directions for further studies.

Table 1.1 lists the scientific production details, such as journal, status, and reference link, as well as the chapter each study referred to.

Table 1.1 - Scientific production.

Title/Link	Journal/ Conference	Status	Chapter
Satellite-based Machine Learning Modelling of Ecosystem Services indicators: A review and meta-analysis	Applied Geography	Published	2
Data-Driven Modelling of Freshwater Ecosystems: A Multiscale Framework Based on Global Geospatial Data	International Conference on Geographical Information Systems Theory, Applications and Management GISTAM 2023	Presented and published	3
A hybrid modelling approach for detecting seasonal variations in inland Green-Blue Ecosystems	Remote Sensing Applications: Society and Environment	Published	4
Climate-driven stock accounts of inland Green-Blue Ecosystems: Coupling the carbon and water cycles via Reverse Engineering and Geodetectors	q1 journal	Under review	5
Revealing dynamics of carbon storage and sequestration in forest ecosystems: A downscaling approach to support monitoring progress towards sustainable management	q1 journal	Under review	6

Published Journal Articles

Almeida, B., & Cabral, P. (2024). A hybrid modelling approach for detecting seasonal variations in inland green-blue ecosystems. *Remote Sensing Applications: Society and Environment*, 33, 1-15. Article 101121. <https://doi.org/10.1016/j.rsase.2023.101121>

Almeida, B., David, J., Campos, F. S., & Cabral, P. (2024). Satellite-based machine learning modelling of Ecosystem Services indicators: A Review and Meta-Analysis. *Applied Geography*. <https://authors.elsevier.com/tracking/article/details.do?aid=103249&jid=JAPG&surname=Almeida>

Published Conference Proceeding

Almeida, B., & Cabral, P. (2023). Data-Driven Modelling of Freshwater Ecosystems: A Multiscale Framework Based on Global Geospatial Data. In C. Grueau, A. Rodrigues, & L. Ragia (Eds.), *Proceedings of the 9th International Conference on Geographical Information Systems Theory, Applications and Management: GISTAM 2023* (Vol. 1, pp. 104-111). SciTePress - Science and Technology Publications. <https://doi.org/10.5220/0012037800003473>

Submitted Journal Articles (Under review)

Almeida, B., Monteiro, L., Scimama, P., & Cabral, P. (2024). Climate-driven stock accounts of inland Green-Blue Ecosystems: Coupling the carbon and water cycles via Reverse Engineering and Geodetectors

Almeida, B., Monteiro, L., & Cabral, P. (2024). Revealing dynamics of carbon storage and sequestration in forest ecosystems: A downscaling approach to support monitoring progress towards sustainable management.

1.3. MATERIALS AND METHODS

1.3.1. Study Area

The study area corresponds to mainland Portugal, which encompasses nearly 90,000 km² of the Iberian Peninsula, located in southwestern Europe. The country's temperate climate reflects influences from both the Atlantic and Mediterranean regions, resulting in cold and wet winters and hot and dry summers (Coelho et al., 2013). The Mediterranean climate is known for its particular regional characteristics: large seasonal contrast in temperature and rainfall (hot dry summers and mild winters), strong wind systems, intense precipitation, and Mediterranean cyclones (Belo-Pereira et al., 2011). Like other Mediterranean regions, Portugal is susceptible to extreme climatic events, such as droughts and desertification effects and is one of the European countries that are most reliant on water resources that originate outside their territory (Almeida & Cabral, 2021). Recent studies have shown evidence of climatic changes, such as the long periods of drought recorded in 1990, 2004/2005 and 2012 (Almeida & Cabral, 2021; Coelho et al., 2013; de Lima et al., 2015; Espírito Santo et al., 2014a). The more frequent occurrence of these events is increasing the severity of seasonality effects on GBE and compromising the provision of services such as freshwater supply, and consequently crop production, and carbon storage and sequestration.

The landscape is highly diverse, with the southern region of the country experiencing water scarcity and higher temperatures, resulting in less exuberant vegetation, contrasting with the more distinct Atlantic and Mediterranean climates found in the north (de Lima et al., 2015). The flat terrain of the southern regions is associated with extensive agriculture and pastures in agroforestry systems that feature low-density evergreen oak trees such as the Cork oak and Holm oak, while higher elevations in the central and northern regions are characterized by small landholdings, family agriculture, and forests of pine and eucalyptus (Costa et al., 2022). Asymmetries in human geography are also evident, with significant human presence and large settlements primarily concentrated along the coast, particularly from the capital city of Lisbon and extending northward (Araya & Cabral, 2010).

The mainland territory is divided into 23 NUTS (Nomenclature of territorial units for statistics) III subregions, 278 municipalities, and 8 river basin districts. The NUTS III classification is a hierarchical scheme designed to divide the economic territory of Europe into smaller geographical regions (Eurostat, 2023). The adoption of these administrative scales is suggested to harmonize human management considerations within the process of demarcation. However, it is essential to recognize that these choices can significantly influence the research findings and conclusions, due to spatial and granularity effects (Turner et al., 1993).

The Tagus Basin in Portugal is the most important source of water in the country due to its productivity, and quality of water (Ribeiro, 1998). The river basin resources are responsible for economic and demographic expansion through the years (Mendonça, 1990). The Lower Tagus Aquifer is in the downstream area of the international river basin districts PTRH5A in Portugal and its correspondence ES030 in Spain. These catchments constitute an important source of water for both Mediterranean countries. With a length of roughly 1000 km and a catchment area of 80,630 km², the Tagus River begins at a height of about 1600 m in eastern Spain and flows into the Atlantic Ocean near Lisbon (Vis & Kasse, 2009). The extensive network drainage promotes easy access to water and supports the development of intensive agriculture (Almeida, 2020), such as annually harvested plants including flooded crops such as rice fields and other inundated croplands, and permanent crops such as vineyards, fruit trees and olive groves (Novo et al., 2018). Forest and seminatural areas are represented by mixed forest and transitional woodland/shrub (Ramos et al., 2017). Due to its strategic location in the surroundings of Lisbon, the most populated region of the country, there is a growing need for changes in land use to develop artificial surfaces such as urban fabric, road and rail networks, airports, dump sites and industrial areas (Mendes et al., 2015), which is compromising water resources and dependent ecosystems in the basin. Precipitation has a seasonal cycle, large inter-annual variability, and periodic episodes of extremely wet or extremely dry years (Coelho et al., 2013). Spring (March through May) contributes 24% of annual precipitation, Summer (June through August) 6%, Autumn (September through November) 28%, and Winter (December through February) 42% (Almeida & Cabral, 2021). This strong seasonality in precipitation results in maximum rainfall extreme occurrences (potentially leading to floods) and relatively frequent extended drought spells (Belo-Pereira et al., 2011). Long drought episodes typically cause agricultural damage and alter water resources Table 1.2 lists the spatial scale, SEO imagery dates and ecosystems assessed in the research stages 2 and 3.

Table 1.2 - Spatial scales, and SEO imagery dates used for ecosystem modelling in research stages 2 and 3.

Stage	Chapter	Spatial Scale	SEO Imagery Dates	Ecosystems
2	3	River Basin District (RBD)/Catchment	25/04/2018; 18/08/2018; 23/08/2018; 29/01/2022	Freshwater & Wetlands
2	4	RBD/Catchment	26/03/2018; 23/08/2018	Terrestrial & Aquatics
3	5	Country	2018	Terrestrial & Aquatics
3	6	Municipality; NUTS III; Country	2018; 2022	Forest (Coniferous & Broadleaves)

1.3.2. Data

1.3.2.1. Satellite Earth Observation data and technologies

Satellite sensors measure the energy that is reflected and emitted from the Earth's surface and translate it into different perspectives, resolutions, and spectral dimensions (Amici et al., 2017). Bands are regions of the electromagnetic spectrum where the sensor acquires

information. These regions depend on the specificities of each sensor, but also the transmissivity of the atmosphere, and are expressed in terms of the measured wavelength limits. The ability of a sensor to distinguish between different ranges of the electromagnetic spectrum defines its spectral resolution. A multispectral sensor has a greater ability to distinguish objects, as it can capture up to a maximum of 20 bands. Different objects from the Earth's surface will interact differently for the same wavelength. This interaction (reflectance) is a function of the composition and texture of each object. The curve of spectral reflectance variation as a wavelength function is called a spectral signature. The typical spectral signature of each material allows the identification of unique objects through satellite imagery.

Radiometric resolution describes a sensor's ability to distinguish objects viewed in the same part of the electromagnetic spectrum. The radiation detected by different sensors is stored in the form of arrays of cells or pixels, with different intensity levels, corresponding to the average of the radiation values recorded over the entire terrain surface represented by the pixel. The radiation intensity measured in each pixel is represented by the DN (Digital Number), which varies between 0 (corresponding to black, the lowest value) and a maximum value, which depends on the radiometric resolution of the image. Most of the optical images acquired by satellite instruments have a radiometric resolution of 8 bits (or higher), with 256 shades of grey. The most recent satellites have been capturing images with a higher radiometric resolution, which allows greater detail in the representation of information (Liu & Mason, 2009). Landsat 8 and Sentinel-2A instruments acquire measurements at 12 bits. These measurements are converted to reflectance and stored as 16-bit integers.

The resolution of the satellite sensors makes it possible to quantify the information acquisition capabilities, from the point of view of the covered electromagnetic spectrum range (spectral resolution), the coverage on the ground (spatial resolution), the frequency of repetition of data acquisition at the same location (temporal resolution) or the number of intensity levels of energy represented in each pixel (radiometric resolution). The spatial resolution of a sensor refers to the dimension of the Earth's surface that is represented by each cell or pixel of the image, called IFOV (Instantaneous Field Of View). This quantity is directly proportional to the distance between the sensor and the observed surface (Lausch et al., 2016). High spatial resolution sensors represent a smaller area of land but with more detail and accuracy (Liang & Wang, 2019). However, higher resolution implies larger files, more loading, viewing, and processing time and more space taken up in databases. The development of big earth data technologies is overcoming these obstacles by optimizing means and processing time.

The SEO data and technologies used in this research are publicly available and recognized as high spatial resolution satellites (5 - 100 m/pixel) (Vyvlečka & Pechanec, 2023), including imagery captured by the Sentinel-2 mission. The European Spatial Agency (ESA, 2022) has already launched more than 70 earth observation satellites into space, including the Sentinel-1 and Sentinel-2 pairs that are part of the Copernicus mission. The programme is designed to include 7 generations of Sentinel satellites/sensors, featuring distinct technologies for monitoring terrestrial, oceanic and atmospheric processes, operating in the radar and multispectral wavebands. Sentinel-1 instruments and Sentinel-2 have been in operation since April 2014 and June 2015 respectively, the first of which collects radar information and the second is a high-resolution multispectral sensor MSI (Multispectral Instrument) that records optical information on vegetation, soil, water, and coastal zones. The MSI sensor installed in

Sentinel-2 acquires and records information in 13 bands: visible (VIS with 4 bands), near-infrared (NIR with 6 bands) and shortwave infrared (SWIR with 3 bands). This instrument can detect small differences in spectral signatures, as they have contiguous bands with small bandwidths (<20 nm). The spatial resolution is 10, 20 and 60 m respectively depending on the band, with a high temporal resolution of 5 days.

At the catchment level, 5 multispectral Sentinel-2 images captured in the Winter, Spring, and Summer seasons of the Mediterranean climate zone, were downloaded from the Copernicus Open Access Hub (<https://browser.dataspace.copernicus.eu/>). Spring and Summer were selected since they are typically the seasons with the lowest average contributions of precipitation, and as a result, less soil water-holding capacity (Belo-Pereira et al., 2011). This is required to distinguish waterbodies from flooded areas (Barron et al., 2014), as major floods that have occurred in the study area since 1980 were throughout the Autumn-Winter season (November to February) (de Lima et al., 2015), and detect the seasonal variation in the greenness of vegetated land (particularly in the Summer) (Doody et al., 2017). The dates were selected based on the percentage of cloud cover, which was less than 5%.

Encompassing the entire mainland of Portugal for the years 2018 and 2022, a total of 1183 and 1154 images, respectively were retrieved through the Google Earth Engine (GEE) (Google, 2023) platform. All available spectral bands from Sentinel-2 imagery were used in data stacks, along with satellite-derived indices.

The combination of algebraic operations in pre-established bands leads to the definition of indices that allow highlighting certain information (i.e., water, vegetation, soil, minerals, etc.). Spectral-derived indices result from combinations of two or more spectral bands designed for the enhancement of specific objects (Kuenzer et al., 2014). The spectral indices employed included the Normalized Difference Vegetation Index (NDVI) (Rouse et al., 1973) and Enhanced Vegetation Index (EVI) (Huete et al., 1997), used to highlight and distinguish vegetation of different types and at different stages of its evolutionary seasonal cycle. Additionally, the Soil Adjusted Vegetation Index (SAVI) (Huete, 1988) was utilized to reduce the impact of soil reflectance and enhance vegetation response. The NDMI was employed as it is an indicator of forest change and water stress that enables capturing the moisture differences between land use types (Silleos et al., 2008). Finally, NDWI was used to distinguish water and soil (Gao, 1996) capturing water only in the areas of the deepest channels and with the cleanest water (Ji et al., 2015). A combination of spectral-derived indices and ancillary data (i.e., climatic, topographic, population density, road network information, number of trees, soil type and geology) is commonly included as predictor variables, in environmental modelling. Aboveground biomass, water yield, and soil moisture content are some examples of ESI that are highly dependent on climatic and topographic drivers such as precipitation, evapotranspiration, temperature, elevation, and slope.

1.3.2.2. Geospatial data

In the scope of this research, a wide range of geospatial datasets were used (Table 1.3). It includes topographic data such as slope and elevation; climatic data such as precipitation, potential evapotranspiration and global aridity index; and a diverse source and type of LULC data. The topographic characteristics including slope and elevation were derived from the Global Digital Surface Model dataset - Advanced Land Observing Satellite-3 (ALOS-3) with a horizontal resolution of

approximately 30-meter mesh, provided by Japan Aerospace Exploration Agency (JAXA, 2023) free of charge. Another considered source of topographic data is NASA through the Shuttle Radar Topography Mission (SRTM). The annual precipitation was obtained from the WorldClim database (Fick & Hijmans, 2017) and the Global Potential Evapotranspiration (Global-PET) and the Global Aridity Index (Global-Aridity) from the Consortium of Spatial Information, Global-Aridity and Global-PET Database (Trabucco & Zomer, 2019). Global data precipitation was obtained from spatial interpolation of nearly 60,000 weather stations providing monthly climate data. The datasets have a spatial resolution of approximately 1 km². Reference evapotranspiration and global aridity were derived from the WorldClim precipitation model and have the same spatial resolution and temporal scale. High-resolution LULC data were derived from the Portuguese LULC map for the year 2018 (COS2018), developed by the Directorate General for Territory (DGT, 2018). The values of carbon density of aboveground biomass (AGB) in each forest class in tons per hectare (t/ha) were compiled from the 6th Portuguese National Forestry Inventory (ICNF, 2023). The Corine Land Cover (CLC) map of 2018 (spatial resolution of 100 m) (Copernicus Programme, 2023) was also considered. Surface water and groundwater bodies datasets are from the European Environment Agency – EEA (EEA, 2023) in a version released in the same year, and the depth of the aquifer is derived from the National Information System of Hydric Resources – SNIRH (SNIRH, 2023).

Table 1.3 - Description of the datasets, their source and pixel resolution.

Data	Source	Cell size	Subject	Scale
Global Digital Surface Model (DSM) (m)	Earth Observation Research Center Japan Aerospace Exploration Agency (JAXA EORC) - GEE	30 m	Topographic	Global
Digital Elevation Model (DEM) (m) & Slope (SLOPE) (%)	NASA Shuttle Radar Topography Mission (https://www.earthdata.nasa.gov/)	30 m	Topographic	Global
Average Annual Precipitation (mm)	WorldClim (https://worldclim.org/)	1 km	Climatic	Global
Global Potential Evapotranspiration (Global-PET) (mm)	Consortium of Spatial Information-CSI (http://www.cgiar-csi.org)	1 km	Climatic	Global
Global Aridity Index (Global-Aridity)	Consortium of Spatial Information-CSI (http://www.cgiar-csi.org)	1 km	Climatic	Global
Land Use Land Cover Map (COS2018) 2018	Directorate General for Territory - DGT (https://snig.dgterritorio.gov.pt/)	10 m	LULC	Country
Corine Land Use and Land Cover 2018	Copernicus Land Monitoring Service - CLMS (https://land.copernicus.eu/)	100 m	LULC	Europe
Groundwater depth 2018	National Information System of Hydric Resources – SNIRH (https://snirh.apambiente.pt/)	-	LULC	Country
Surface water and groundwater bodies	European Environmental Agency - EEA (https://www.eea.europa.eu/)	-	LULC	Europe
Water & Wetness Probability Index (WWPI %) 2018	Copernicus Land Monitoring Services - CLMS (https://land.copernicus.eu/looking-for-national-products)	10 m	LULC	Europe
Tree Cover Density (TCD %) 2018	Copernicus Land Monitoring Services - CLMS (https://land.copernicus.eu/looking-for-national-products)	10 m	LULC	Europe
Carbon density (t/ha)	Institute of Nature and Forest Conservation - ICNF (https://www.icnf.pt/)	-	Portuguese National Forestry Inventory	Country

The WWPI is a raster displaying the occurrence of water and wet areas as an index on a scale between 0 (only dry observations) to 100 (only water observations) (Copernicus Programme, 2023). It indicates the degree of wetness in a physical sense, independently of the actual vegetation cover. The landscape elements included in the datasets are permanent and temporary open water bodies, temporarily inundated areas, wet agricultural fields, and transitional coastal water bodies (European Environment Agency, 2023). TCD provides continuous-scale (0-100%) information on crown cover for the whole of Europe. Apart from mapping the current status, it is used to monitor changes, and map losses and gains of tree cover. Similar to the WWPI, it is part of the Copernicus High-Resolution Layers portfolio, providing detailed information across Europe through a wide variety of geospatial datasets developed based on satellite data.

1.3.3. Data-driven modelling through Machine Learning

Data-driven approaches provide the foundation for data analysis and interpretation, while ML algorithms are the tools to build predictive models and automate decision-making processes through learning from data (Craven et al., 2023). An ML algorithm performs tasks that improve with experience, i.e. learning, in a way that its behaviour is constantly being measured (James et al., 2013). A learning system can improve in different ways, such as by analogy modifying knowledge from one domain to build intelligence in another domain, learning from examples in a supervised way, most related to classification tasks, learning by doing, by being told, learning from detecting patterns, and clustering in unsupervised learnings. In supervised learning (SL), the training data is known and labelled, allowing to improve the learner's performance directly. In unsupervised learning (UL) all data are unlabelled, and the machine learns to find structure and new features in the data. UL has the advantage that doesn't require training samples, but its accuracy is quite low compared to supervised methods, which rely on training samples to establish the relationships between inputs and results (Q. Wang et al., 2019). If the values are continuous, it's a regression problem that will fit the data as closely as possible to predict continuous values. If the values are discrete, it's a classification problem that will find the discriminant between discrete classes. In ML models the targets are the response variables, also known as dependent variables.

A typical ML algorithm starts with the identification of an expected output or task that must be performed, then the element that will provide the experience to the learning system (training data) is presented, and finally, the interaction between the task and training data requires a third element, that measures the performance of the learning process (Domingos, 2012). The necessary data to implement a learning machine process is commonly divided into training, validation, and test datasets. The training data are the predictors, the validation dataset is used to control the learning process and the test dataset is employed to assess the learner's performance (Hastie et al., 2009). ML algorithms were introduced in satellite imagery processing due to their ability to manage high-dimensional data and map classes with extremely complex properties, without making statistical assumptions about data distribution (Tyler et al., 2016). Methods most used to model complex class signatures are support vector machines (SVM), decision trees (DT), Random Forests (RF), boosted DT, artificial neural networks (ANN), and k-nearest neighbours (k-NN) (Maxwell et al., 2018). Nowadays many other algorithms are being widely adopted, as computational processing is being developed, and the already-known techniques have been improved. Classification and regression tasks were performed in the research stages 2 and 3 (Table 1.4). In research stage 3, both studies were processed, analysed and modelled in the Google Earth Engine (GEE) platform.

Table 1.4 - ML tasks, algorithms, targets and metrics.

Research Stage	Chapter	Task	Algorithm	Target	Accuracy Assessment
2	3	Regression	Decision Trees (DT)	Water & Wetness Probability Index (WWPI)	Coefficient of determination (R-squared) and regression error (Re)
2	4	Binary & Multiclass Classifications	Support Vector Machines (SVM); DT; Convolutional Neural Networks (CNN)	Terrestrial & Aquatics (GBE)	Accuracy, Recall, Precision, F1-score, ROC-AUC
3	5	Binary & Multiclass Classifications; Regression	RF; DT	GBE; WWPI; TCD	OA, PA, UA, K Confusion matrix, F1 score; R-squared, Re
3	6	Binary & Multiclass Classifications	SVM	Forest (Coniferous & Broadleaves)	Overall Accuracy (OA), Producer Accuracy (PA), User Accuracy (UA), Kappa coefficient (K)

STAGE 1: RESEARCH CONCEPTUALIZATION AND DESIGN

As new techniques and data are forthcoming more frequently the existing studies are becoming out of date rapidly. Systematic reviews related to RS technologies and satellite missions are quickly being replaced by novelty. Very often, new findings, tools, and research are being developed to bring advanced knowledge to the scientific community and society. Through meta-analysis, an overwhelming volume of research can be reduced without loss of quality on results. Systematic reviews provide reproducibility and transparency for the scientific community, and decision-makers, aggregating and synthesizing findings or evaluating hypotheses. Research stage 1 goal was to provide baselines for further stages 2 and 3 through reviewing studies that have developed satellite-based ML models to assess ESI. Studies were thoroughly analyzed concerning the location, spatial and temporal scales, satellite, and sensor data used, ES assessed, applications, the methodology employed, and overall outcomes and limitations. The purpose of this systematic study was to summarize ML models developed to assess ES and analyze their relationship, adopting a methodology that enables users to evaluate, repeat or revise the review's findings.

Almeida, B., David, J., Campos, F. S., & Cabral, P. (2024). Satellite-based machine learning modelling of Ecosystem Services indicators: A Review and Meta-Analysis. *Applied Geography*. [10.1016/j.apgeog.2024.103249](https://doi.org/10.1016/j.apgeog.2024.103249)

2. SATELLITE-BASED MACHINE-LEARNING MODELLING OF ECOSYSTEM SERVICES INDICATORS: A REVIEW AND META-ANALYSIS

2.1. INTRODUCTION

Nature offers society a diverse array of services and resources through Ecosystem Services (ES) (Costanza et al., 1997). Natural ecosystems, recognized for their ability to deliver a multitude of ES, are appraised as assets through physical and monetary evaluations recorded as stock and flow accounts (Vallecillo et al., 2019). The physical accounts involve quantifying ecosystem extent, measuring the total occupied area, and assessing indicators that reflect the conditions of ecosystems and their services (Edens et al., 2022b). ES indicators (ESi) are measurable parameters that provide insights into the status and trends of the diverse benefits ecosystems offer to humanity, spanning ecological, economic, and social dimensions, as well as for making policy and management decisions (Olander et al., 2018). The aboveground and belowground biomass in forests plays a crucial role in supporting water filtration services by collecting and filtering rainfall before it reaches streams and rivers. ESi, such as tree cover density, water and wetness probability index, and soil depth, serve as proxies to describe the status of the water filtration service, contributing to providing cleaner water and reducing water treatment costs (United Nations et al., 2021).

Therefore, assessing ESi is still a challenge due to the intricate relationships within ecological dynamic systems, which involve numerous processes and components that interact nonlinearly (Haines-Young & Potschin, 2012). Besides, traditional approaches relying on simplistic spatial surrogates, often lead to incomplete representations of biophysical variables, and extensive ground surveys for spatially explicit mapping encounter limitations such as high costs and scale restrictions (Zergaw Ayanu et al., 2012).

The literature proposes various methods to quantify ESi and natural stocks (Boyd & Banzhaf, 2007; De Groot et al., 2002; Fisher et al., 2009; Kienast et al., 2009; Syrbe & Walz, 2012). These studies have emphasized the importance of taking a comprehensive and integrated approach to developing and implementing ESi. A frequently employed approach involves extrapolating measurements of landscape ability provisioning through the utilization of land use and land cover (LULC) maps (Bolliger & Kienast, 2010; Costanza et al., 1997). Previous reviews (Andrew et al., 2014; de Araujo Barbosa et al., 2015; Feng et al., 2010; Malinga et al., 2015; Martínez-Harms & Balvanera, 2012; Zergaw Ayanu et al., 2012) have remarked that the main proxies for mapping ES, monitoring environmental status, and assessing ecosystems' extent and conditions often involve LULC variables.

However, limitations persist in accurately quantifying the interconnections among ecosystem functions, services, and the benefits to human well-being (Cord et al., 2017; Lausch et al., 2016). Ramirez-Reyes et al. (2019) emphasized the importance of shifting from categorical to continuous conceptualization in modelling ESi, as parameter coefficients are generally derived from field research or literature reviews. An alternative approach extending beyond mapping the presence/absence of ecosystems or relying on lookup tables for analysis is to use statistical regression to connect in-situ

information with remotely sensed data to quantify ecosystem structure and functional traits (Lobert et al., 2021).

Remote Sensing (RS) offers a distinctive opportunity to systematically assess ecosystems' status across diverse spatial and temporal scales (Skidmore et al., 2021), holding promise for robust monitoring mechanisms within the framework of global sustainability policies and governance (Braun et al., 2018). Particularly Satellite Earth Observation (SEO) emerges as a cost-effective solution, providing data for quantifying and mapping ESI (Vývlečka & Pechanec, 2023). ESI derived from SEO data models are spatial proxies aiding in the ES assessments through measurements of ecosystem extent and conditions (Czúcz et al., 2021).

Recently, Schirpke et al. (2023) conducted a review of studies exploring the use of emerging technologies in ES assessments, revealing the increased application of passive Earth observation sensors and ML algorithms among other technologies. Their study pointed out that in the last decade, ES modelling based on open-access satellite data predominantly involved high and middle spatial resolution sensors (ranging from 10 m to 1 km), such as those on board the Landsat, Sentinel, and Terra/Aqua MODIS satellites. In their review, Vývlečka and Pechanec (2023) showcased a preference for Sentinel-2 over Landsat 8, especially in larger scales and vegetated areas, highlighting the relevance of spatial, temporal, and spectral resolutions in influencing modelling accuracy. They emphasized that additional factors like imagery processing, algorithm selection, and validation data also played crucial roles, and these should be further explored to enhance the potential of applications.

The integration of SEO data and ML stands as a powerful approach for ES assessment across multiple scales (Liang & Wang, 2019; Y. Wang et al., 2021; Willcock et al., 2018). ML has become crucial in environmental and landscape modelling, particularly in leveraging satellite data to precisely map diverse landscape properties (Ez-zahouani et al., 2023). They serve as a powerful tool for addressing challenges related to data-sparse locations, providing efficient estimations, and accounting for uncertainties in modelling ESI (Scowen et al., 2021). ML algorithms, such as Support Vector Machine (SVM) and Random Forest (RF), are widely used in RS applications (Maxwell et al., 2018), whereas Deep Learning (DL) has emerged as an advanced technique excelling at discriminating complex and nonlinear data structures (Goodfellow et al., 2016; LeCun et al., 2015) with great potential to fostering environmental modelling based on RS data (Ma et al., 2019; Pritt & Chern, 2018).

Various methods, including SVM, Decision Trees (DT), RF, Artificial Neural Networks (ANN), and k-Nearest Neighbours (k-NN), are widely utilized to predict complex LULC classes (Maxwell et al., 2018). Additionally, ensemble methods like Gradient Boosting, CatBoost, and Stochastic Gradient Boosting are adopted to enhance predictions (Friedman, 2001; Prokhorenkova et al., 2017). Thus, ML offers a feasible means to assess ecosystems' status, handling large and multidimensional datasets without relying only on oversimplified approaches or algorithms (Willcock et al., 2018). Despite the potential benefits, the implementation of SEO data and ML in ES research remains limited, posing some constraints (Czúcz et al., 2021). Challenges persist in refining methods, such as model settings, conceptualization, and knowledge of ecosystem influential factors, underscoring the need for ongoing research development (Kubiszewski et al., 2022).

Recent literature reviews were focused on unveiling technologies for overcoming limitations encountered in ES assessments: Manley et al. (2022) showcased the current application of ML and Big Data to tackle gaps related to data availability, uncertainty understanding, and socio-environmental

connections. Scowen et al. (2021) conducted a review to investigate the utilization of ML in ES research and identify trends in ML approaches. Their findings revealed that ML techniques are applied in data description and predictive modelling in a variety of datasets, including RS data from satellites and aerial vehicles. Other studies have contributed to the field of ES mapping and monitoring through RS, such as Feng et al. (2010), exploring the role of RS in ES assessments. Zergaw Ayanu et al. (2012) reviewed RS systems, sensor types, and methodologies relevant to quantifying provisioning and regulatory ESi. Andrew et al. (2014) explored the capabilities of RS in describing biodiversity, plant traits, and various ecological variables, emphasizing their contributions to ES assessments. Lausch et al. (2016) highlighted the affordability and repeatability of Earth Observation methods for measuring taxonomic, functional, and structural diversity. They called for a systematic approach to cross-case comparisons and methods development. Pettorelli et al. (2018) addressed the lack of consensus on defining and tracking ecosystem functions beyond the site level, proposing a framework for worldwide monitoring using satellite RS. C. Ramirez-Reyes et al. (2019) organized a workshop with researchers and decision-makers to outline stages in the assessment process where SEO could be applied. Their findings stressed that the widespread adoption of SEO data and technologies in ES assessments requires addressing conceptual barriers, including adapting existing products and models to accommodate continuous data.

Regardless of existing studies researching ES assessments through RS and ML, there is a gap in understanding the satellite-based ML modelling components, such as instruments, data integration, type of analysis and assessments, modelling conceptualization, development, and implementation. In this review article, we aim to offer a comprehensive overview of the current state of research in this domain, providing a synthesis of key methodologies, and answering the following research questions: i. Which SEO data are used for modelling ESi? ii. Which ESi are assessed using SEO and ML techniques? iii. Which ML models are implemented? iv. What is the relationship between ML tasks and ESi? v. Is there a rule for model development within ESi?

To address these questions, a systematic literature review and meta-analysis are conducted following the PRISMA 2020 (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) (Page et al., 2021) guidelines covering the literature from 2012 to 2022, and applying content analysis to formulate assumptions tested through statistical analysis. The review process utilizes a meta-analytical approach to understand the ML tasks applied to model ESi, providing a further understanding of the satellite-based ML modelling components such as SEO technologies, instruments, data integration, and type of analysis and assessments. Major outcomes incorporate insights into the application of SEO data and ML in ESi modelling, contributing to advancing the knowledge of the latest approaches developed by researchers worldwide.

2.2. MATERIALS AND METHODS

Systematic reviews play a role for scholars and decision-makers, offering a structured approach to navigate through the vast volume of research and providing a solid foundation for informed decision-making (Greco et al., 2013). A systematic review process requires adhering to a set of baselines to identify, select, and synthesize data from the literature, enabling users to evaluate, reproduce, or

update the findings (Higgins & Thompson, 2002). Our study follows the methodology schema presented in Figure 2.1. The process includes conceptualization and research design, search strategy and data collection, data processing, content analysis, synthesis of results, and discussion.

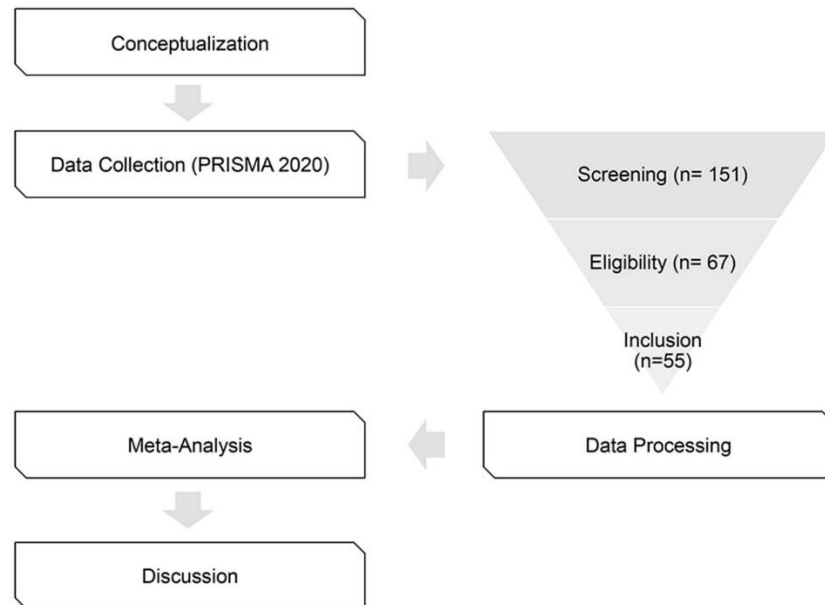


Figure 2.1 - Diagram flow of the meta-analytic reviewing process. n refers to the number of studies selected in each phase.

2.2.1. Research Design

A top-down strategy was used in the problem conceptualization to break down the study into keywords, associated terms, and synonyms, considering the different ways of spelling. This step is crucial for defining the research concepts and constructing the search query.

The research design followed the building blocks of theory development proposed by (Whetten, 1989), including the essential elements for a phenomena explanation: *what*, *how*, *why*, *when*, *who* and *where*. A top-down strategy was used in the problem conceptualization to break down the research into keywords, associated terms, and synonyms, considering the different ways of spelling. This step is crucial for defining the research concepts and constructing the search query. Individual components of the problem are specified in detail at this step, and composition takes place. *What* and *how* questions helped to bring out the keywords and associated terms related to ES, SEO data (checked for Sentinel, and all missions of Landsat), and ML techniques. The *why* asks for the purpose of developing such models, *when* asks for the temporal scale of studies to be analyzed, *who* identifies the authors, and *where* flags the study's location. The building blocks for the research design and for building the search query are well detailed in Figure 2.2.

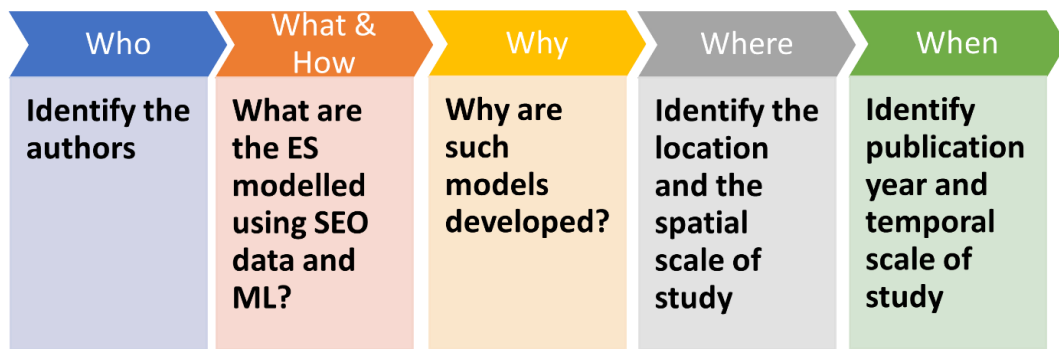


Figure 2.2 - The building blocks for the research design and for building the search query.

2.2.2. Search Strategy and Data Collection

An objective search strategy was implemented to identify the most relevant studies in the research scope. The Scopus scientific database (Elsevier B.V, 2023) was the source of the scientific literature and was last queried on 30/09/2022. The data collection process comprises four main phases. Phase one, identification, starts with the application of the search query to identify studies. As the search terms must be logically connected, the search mechanism applied advanced techniques to the query-building process such as Boolean operators, quotes, stop words, wildcards, and nesting. The OR operator is used to aggregate similar concepts (synonyms or associated words), while the AND operator is applied to narrow the results. To search for specific phrases, the terms must be enclosed in double quotes (") or, for an exact match inside braces ({}). In Scopus, the operator OR has precedence to AND, i.e., first, the Scopus searching algorithm processes the OR connector by looking for documents containing the specified words, and last processes the AND operator, by returning any documents it finds. Besides, the following assumptions were considered: 1) The stage of publication should be set to Final; 2) The types of documents are limited to articles published in a scientific peer-reviewed journal; 3) The publication must be written in the English language; and 4) The search is within article title, abstract and keyword (TITLE-ABS-KEY). These assumptions are expressed by reserved words from the Scopus search, i.e., LIMIT-TO (limits the search to the assumptions), DOCTYPE (refers to the type of document that can be an article, a review, or a book), PUBSTAGE (publication stage that can be final or article in press), PUBYEAR (is the year of publication), and SRCTYPE (refers to the publishing source). The search strategy implemented in Scopus is detailed in Table 2.1. A total of 151 studies were identified by the query.

Table 2.1 - Data Collection: Scopus searching query.

Scopus searching query
TITLE-ABS-KEY (({ecosystem service} OR {ecosystem services} OR (ecosystem-service*) OR (ecosystem* AND (demand* OR suppl* OR account* OR bundl* OR flow* OR value* OR function*)) OR {natural capital}) AND ((remote AND sens*) OR satellite* OR {earth observation} OR {big earth data} OR sentinel* OR sensor* OR {landsat} OR {imagery} OR {remotely sensed} OR {big-data}

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) AND ( monitor* OR map* OR observ* OR detect* OR predic* OR classif* ) AND ( landscape* OR
inland OR terrestr* OR natur* OR biophysi* OR socio-ecological ) AND ( metric* OR indic* OR
index* OR prox* OR tradeoff* OR trade-off* OR footprint* OR parameter* OR variable* ) AND (
{spatiotemporal} OR {spatiotemporal} OR {spatiotemporal} OR {spacetime scales} OR
{spatiotemporal scales} OR {spatiotemporal} OR spati* OR temp* OR time* ) AND ( *machine* OR (
machine-learning ) OR ( artificial-intelligence ) OR *learning* ) ) AND ( PUBYEAR > 2012 ) AND (
LIMIT-TO ( SRCTYPE , "j" ) ) AND ( LIMIT-TO ( PUBSTAGE , "final" ) ) AND ( LIMIT-TO ( DOCTYPE , "ar"
) OR LIMIT-TO ( DOCTYPE , "re" ) ) AND ( LIMIT-TO ( LANGUAGE , "English" ) )

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Phase 2, screening, consisted of analysing the abstracts of 151 records. In this phase, we assessed if the identified studies developed a model that is: 1. addresses one or more types of ES; 2. using Sentinel-2 and/or Landsat imagery; and 3. applying ML techniques. In the end, 67 records were selected to be full-text analysed. In phase 3, eligibility, the studies were excluded if their content did not fulfil requirements 1, 2, and 3, which led to the exclusion of 12 records. In the fourth phase, inclusion, a total of 55 articles were included in the systematic review process. A complete list of the selected studies is provided in the A2. Appendix - Chapter 2, Table A2.1.

2.2.3. Content Analysis and Synthesis

The process of acquiring information began with content analysis and a summary of findings. Qualitative data were synthesized and processed for statistical analysis. The content examination included: 1) presenting where the selected studies were implemented and when they were published; 2) confirming the use of Sentinel-2 and Landsat missions within studies; 3) summarizing Biomes, ecosystems categories, and services; 4) identifying the ML algorithms (learners) employed, the tasks (classification or regression) carried out, and the evaluation metrics used to assess models uncertainties; 5) synthesizing modelling purposes, common limitations, and opportunities argued in the studies. To exemplify these key points and establish connections between them, we referred to specific examples from the selected literature.

Table 2.2 depicts current operational Landsat and Sentinel missions most applied to Earth monitoring services. NASA's Earth Observing System (NASA's EOS, 2022) comprises a coordinated constellation of satellites encompassing more than 20 missions. Notably, the Landsat satellites, operated jointly by NASA and the U.S. Geological Survey, represent the initial and most enduring terrestrial observation program focused on monitoring natural resources. Since 2009, all Landsat images have been made accessible to the public at no cost, contributing to open and widespread access to valuable SEO data (NASA, 2023).

The Landsat 1 was launched in 1972 and was the first satellite of this program, which has been continuously improved over the last four decades, Landsat 9 was the last one launched (2021). Landsat 7 mission started in 1999 carrying the ETM+ (Enhanced Thematic Mapper Plus) sensor, which includes a thermal infrared band (TIR) with a spatial resolution of 60m. While Landsat 7 is still operational, it is in end-of-life activities. Landsat 8 was launched in 2013 and was equipped with two sensors: the OLI (Operational Land Imager) and the TIRS (Thermal Infrared Sensor). The OLI sensor produces images with 30m spatial resolution in the Visible (VIS), Near Infrared (NIR), and Short-Wave Infrared (SWIR) bands (in 8 distinct bands), and a panchromatic image with a resolution of 15m, the TIRS sensor records

thermal images with a resolution of 100m. The enhancements introduced in Landsat 9 encompass higher radiometric resolution for OLI-2, enabling sensors to discern more nuanced differences, particularly in darker areas like water bodies or dense forests. Furthermore, TIRS-2 has substantially minimized stray light in comparison to its predecessor facilitating improved atmospheric correction and surface temperature measurements.

The European Space Agency (ESA, 2022) has successfully deployed over 70 Earth observation satellites into space. Among them, the Sentinel-1 and Sentinel-2 pairs are integral components of the Copernicus mission. This program is structured to encompass seven generations of Sentinel satellites equipped with specific technologies tailored for monitoring terrestrial, oceanic, and atmospheric processes. The Sentinel missions operate in both radar and multispectral wavebands, providing data for a range of Earth observation applications. Sentinel-1 and Sentinel-2A have been operational since 2014 and 2015 respectively, the first of which collects information through a Synthetic-aperture radar (SAR) sensor, and the second has a multi-spectral instrument (MSI) capturing optical information. Sentinel-2A/2B missions record information in 13 bands: VIS with 4 bands, NIR with 6 bands, and SWIR with 3 bands. The spatial resolution is 10, 20, and 60m, respectively, depending on the band, with a temporal resolution of 5 days. As many studies did not distinguish between Sentinel-2A and 2B data, this review grouped Sentinel-2A and 2B into Sentinel-2. The same happened for Sentinel-1.

Table 2.2 - Most operational Landsat and Sentinel missions applied to Earth monitoring services.

Mission Name	Mission Agencies	Launch Year	End-Of-Life Year	Applications	Instruments
Landsat 7	USGS, NASA	1999	2024	Earth resources, land surface, environmental monitoring, agriculture and forestry, disaster monitoring and assessment, ice and snow cover.	ETM+
Landsat 8	USGS, NASA	2013	2028		OLI, TIRS
Landsat 9	USGS, NASA	2021	2031		OLI-2, TIRS-2
Sentinel-1A	ESA	2014	2024	Monitoring of sea, ice zones, and the arctic environment, surveillance of marine environment, monitoring of land surface motion risks, and mapping in support of humanitarian aid in crises.	C-Band SAR
Sentinel-2A; 2B	ESA	2015; 2017	2025; 2027	Land monitoring-related services: generation of land cover maps, risk mapping, disaster relief, generation of leaf coverage, leaf chlorophyll content, and leaf water content.	MSI (Sentinel-2)

In satellite-based applications, ML techniques are frequently employed for classification and regression problems (Ma et al., 2019). The targets are the response variables, also known as dependent variables; if the values are continuous, it is a regression problem that will fit the data as closely as possible to predict continuous values. Such as the prediction of tree cover density and leaf area index, as proxies for timber production included in the provision of raw materials service (Cilek et al., 2022; Mallinis et al., 2020), or the predictions of water and wetness probability index as a proxy for water provision and wetlands (Almeida & Cabral, 2023; Ludwig et al., 2019). If the values are discrete, it is a classification problem that will find the discriminant between discrete classes.

As many studies performed classification tasks without considering a recognized nomenclature to categorize ESi, we adopted the grouping system proposed by The Economics of Ecosystems and Biodiversity (TEEB) valuation database (McVittie & Hussain, 2013). TEEB provides a valuation framework to assist decision-makers in examining the impacts of international and national policies on biodiversity and ecosystems. Compared with other ES categorization systems, TEEB puts together habitat and supporting services to avoid the double-counting problem (Mustajoki et al., 2020).

ESi were categorized into four main functioning groups: (1) production functions, contributing to provisioning services; (2) regulation functions, involved in supplying regulating services; (3) habitat functions, essential for preserving ecological structures and processes, thereby offering supporting services; (4) cultural functions, delivering cultural and amenity services (Kienast et al., 2009).

ESi was employed, acknowledging their varied names under different categorization systems. Indicators were renamed and grouped as ESi based on the parameters or proxies mapped, not just the terms used in the original papers, as they varied considerably. We expand our typology to encompass biodiversity, recognizing its frequent treatment as an ES in the literature review. Since many records considered biodiversity in terms of genetic, functional, or habitat diversity, we follow this rationale, placing it in the habitat/supporting category. For instance, leaf coverage and leaf chlorophyll content act as indicators for climate regulating services (Egoh et al., 2012), the assessment of genetic resources serves as a measure of biodiversity (King et al., 2021), soil organic matter content functions as a proxy for soil formation and nutrient cycling (Vasenev et al., 2018), and water yield serves as an indicator for water provisioning service (Ludwig et al., 2019).

Meta-analysis uses statistical techniques to synthesize findings in a systematic review (Copas & Shi, 2000). Most meta-analysis methods are developed to measure variations across studies, improve research confidence, answer explicit questions, assess controversies in studies, and generate new hypotheses (Higgins et al., 2022). The log response ratio (logRR) (Hedges et al., 1999) was used to calculate the effect size of studies that developed ML models to assess ESi. Response ratio investigates weighted variance within groups, and the effect size estimates the change in the means in each ES (Durlak, 2009). The Q-test for heterogeneity (τ^2) (Cochran, 1954) and the I^2 statistic (Higgins & Thompson, 2002) were calculated to quantify variation across studies. Overall, this meta-analysis aimed to build evidence on the use of ML models by each group of ES. The main outcome is to evaluate the general applicability of employing hybrid models including classification and regression tasks instead of just one of them. The analysis was carried out using the R Studio software (R Core Team, 2022), through the “metafor” package version 4.0.0 (Viechtbauer, 2010).

2.3. RESULTS

2.3.1. Location of studies

One of the reviewed studies had a global scope, while other studies covered 26 different countries within the selected literature. Studies locations were grouped into six categories according to the number of studies carried out in each country (Figure 2.3). China and the United States of America (USA) gathered the highest number of studies with seven and ten studies, respectively. Bangladesh and India contributed with four and five studies, respectively. Brazil, Germany, Greece, and Spain had three selected studies, followed by other countries including, Italy, Kenya, Peru, Portugal, and South Africa, contributing two studies each. The remaining countries had one study each.

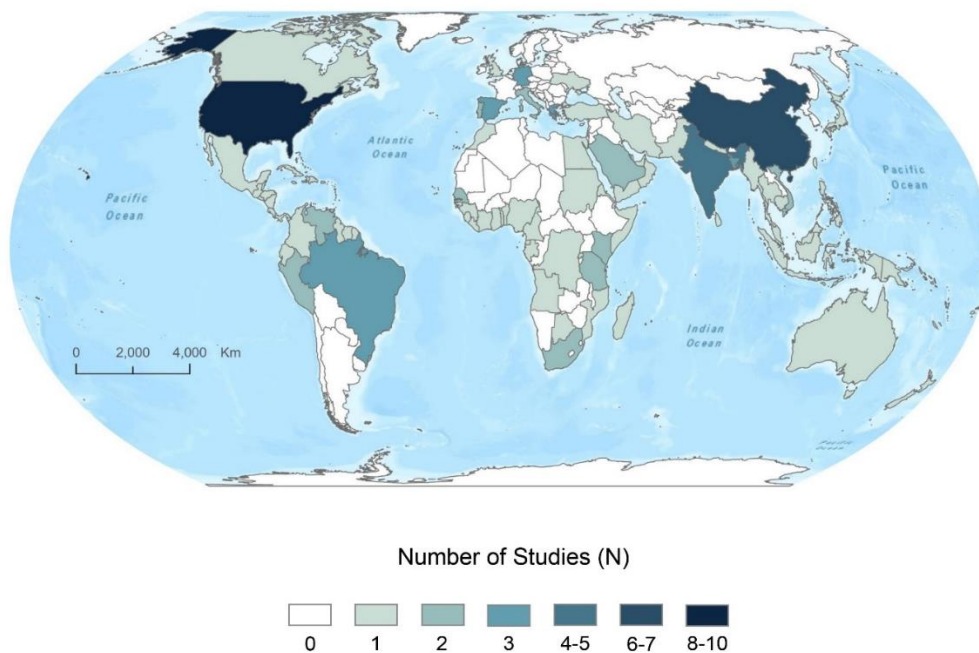


Figure 2.3 - Global representation of the studies included in the review.

The global scale research of Sanderman et al. (2018) includes an ML model to map mangrove forest soil carbon at 30m spatial resolution. Six other studies were applied to more than one country as they were assessing transboundary ecosystems. All countries reported in the reviewed literature were taken into consideration when producing the above global map. Boutsoukis et al. (2019) developed an ML model to estimate the canopy in temperate forests of Germany and the Czech Republic; Guio Blanco et al. (2018) estimated soil water retention in Venezuela and Peru; Koskikala et al. (2020) mapped natural forest remnants in Tanzania and Kenya; Kundu et al. (2022) predicted induced wetland fragmentation and water richness in dams of India and Bangladesh; Mpakairi et al. (2022) estimated

vegetation heterogeneity within arid environments in Botswana and South Africa, and Sannigrahi et al. (2019b) assessed coastal resources values in India and Bangladesh.

Among the selected studies, the earliest publishing dates go back to 2015. It relates to a work carried out in Alaska-USA proposing an ML model to estimate a spatial proxy for climate regulation services assessing carbon stored and sequestered in near-surface permafrost (N. J. Pastick et al., 2015). The authors, used Landsat imagery as predictors in a decision tree model, advancing the application of multitemporal SEO data and benchmarking a transition between methods and technologies. For the years 2012, 2013, 2014, and 2016, none of the records fulfilled the proposed eligibility criteria to be included in this review.

2.3.2. Satellite Earth Observation data: Sentinel-2 and Landsat missions

The SEO data and technologies investigated in this research are publicly available and recognized as high spatial resolution sensors (5 - 100 m/pixel) (Liang & Wang, 2019) on board the Landsat (4, 5, 7 and 8) and Sentinel-2 (including 2A/2B) satellites. The following chart (Figure 2.4) synthesizes the use of data from Landsat instruments and Sentinel-2, depicting also studies that used data from multiple sensors represented in the “Other” category.

Since 2017, at least one study has used data from Landsat 4 and 5, whereas in 2019 there were eight. Within studies, Landsat 8 was first used in 2017, and it was used 30 times until 2022. Sentinel-2 has been used 24 times since 2018. Implemented together, they are a powerful source of spatiotemporal information for ESI monitoring purposes (Vývlečka & Pechanec, 2023). Mo et al. (2018) is the only study that used data from all Landsat sensors as well as the Sentinel-2. About 53% of reviewed studies used SEO data from more than one instrument, such as developing research combining data from MSI and OLI-TIRS sensors (Koskikala et al., 2020; Lobert et al., 2021; Mallinis et al., 2020; N. Pastick et al., 2018).

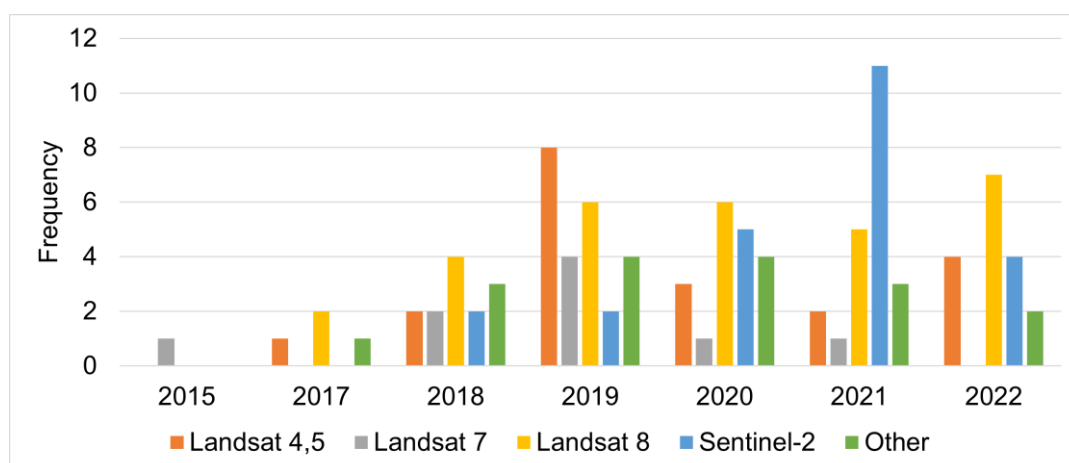


Figure 2.4 - Frequency of SEO data source identified in the literature review. The “Other” category refers to other satellites and instruments combined with any Landsat missions or Sentinel-2.

The “Other” category represents studies that included data from different satellites and instruments, such as combining Sentinel-2 and/or Landsat with radar imagery from Sentinel-1 (DeLancey et al.,

2019a; Hoffmann et al., 2022; Koskikala et al., 2020; Lobert et al., 2021) and other RS technologies such as manned and unmanned aerial vehicles (Hasan et al., 2021; Morell-Monzó et al., 2020; Sharma et al., 2018). DeLancey et al. (2019) highlighted that the combination of optical and radar data provides the highest potential for accurate and comprehensive landscape assessments through satellite-based modelling.

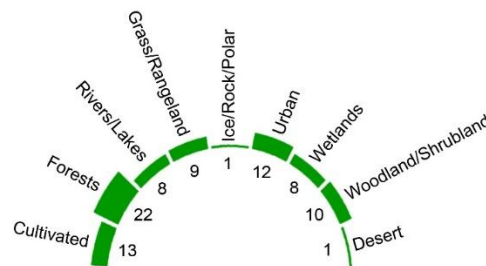
Many other studies combined drone imagery with data from other satellites such as Aqua/Terra MODIS (Moderate Resolution Imaging Spectroradiometer) (Arruda et al., 2021; Mo et al., 2018; Osborne & Alvares-Sanches, 2019a; N. Pastick et al., 2018; Y. Wang et al., 2017; J. Zhang et al., 2019), TripleSat (Cilek et al., 2022), IceSat-2 (Ice, Cloud and land Elevation Satellite) (Narine et al., 2019), SPOT-6 (Satellite pour l'Observation de la Terre) (Sharma et al., 2018), PlanetScope (Leroux, Falconnier, Diouf, Ndao, Gbodjo, Tall, Balde, Clermont-Dauphin, Bégué, Affholder, & Rounsard, 2020), Rapid Eye (Hasan et al., 2021; Leroux, Falconnier, Diouf, Ndao, Gbodjo, Tall, Balde, Clermont-Dauphin, Bégué, Affholder, & Rounsard, 2020; Mallinis et al., 2020), and WorldView-2 (Hasan et al., 2021; Mallinis et al., 2020). Additionally, spectral bands, derived indices, and a wide array of socio-biophysical variables (i.e., climatic, topographic, population density, road network information, census data, soil type, and geology) were considered as features by a few studies (Agrillo et al., 2021; Fitts et al., 2021; Hauser et al., 2021; Hudak et al., 2020; Mallinis et al., 2014; Mouta et al., 2021; Mpakairi et al., 2022c; Nzuza et al., 2021; Pipia et al., 2021; Pizarro et al., 2022; Vidal-Macua et al., 2020a).

2.3.3. Which ESI are assessed using ML techniques?

A considerable number of the studies that performed classification tasks did not use any recognized system to classify ecosystems. Hence before the statistical analysis, we standardized all the classes following the TEEB database framework which recognizes 12 biomes, Marine/Open Ocean, Coastal systems, Wetlands, Rivers and Lakes, Forests, Woodland and shrubland, Grassland, Cultivated, Desert, Tundra, Ice, Rock and Polar, and Urban areas; and 22 ES grouped into 4 main categories: provisioning, regulating, habitat/support and cultural services. The most classified ecosystems were Forests (22), followed by Cultivated lands (13), Urban areas (12), Woodland and shrubland (10), Grass/Rangeland (9), Rivers and lakes, and Wetlands (8) (Figure 2.5a).

Rivers, lakes, and Wetlands were mostly assessed regarding anthropogenic pressures affecting aquatic ecosystems. Kundu et al. (2022) estimated hydro-period, water depth, and water presence consistency, after classifying lakes, rivers and wetlands. Sannigrahi et al., (2019a) developed a model to assess mangrove ecosystems, based on the LULC dynamics. Alqadhi et al. (2022) assessed the impact on ES valuation of future landslide events, from detecting changes in Grass/Rangeland, Urban, Cultivated, Ice/Rock/Polar, Desert, and Rivers and Lakes; Mpakairi et al. (2022) implemented a model to classify the presence of woodland as a proxy for timber production. Gwal et al. (2020) classified natural forests to estimate biomass density; Han et al. (2022) estimated carbon storage through the spatiotemporal dynamics of vegetation, classifying land use into six types: Cultivated, Woodland and shrubland, Grass/Rangeland, Urban, Rivers and Lakes and Wetlands. Morell-Monzó et al. (2020) assessed crop yield for monitoring cultivated lands and maximizing food production and water use. The ES categories with more ML models developed were regulation (35%), followed by provision (29%), habitat/support (25%), and Cultural (12%) (Figure 2.5b).

a) Ecosystems



b) ES indicators

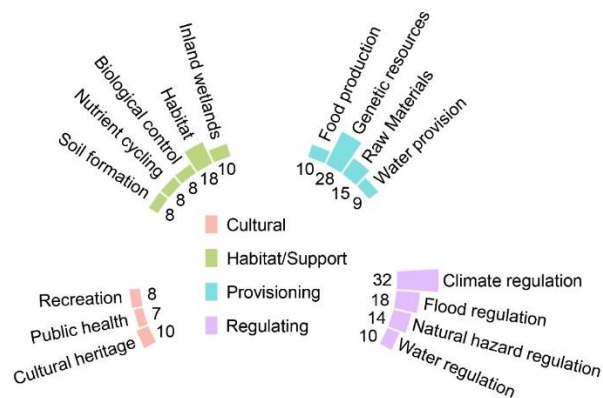


Figure 2.5 - a) Ecosystems and b) Ecosystems categories and services (ESi) modelled by studies.

A total of 16 ESi were identified in the review (biological control, climate regulation, cultural heritage, flood regulation, food production, genetic resources, habitat, inland wetlands, natural hazard regulation, nutrient cycling, public health, raw materials, recreation, soil formation, water provision, water regulation). Within the regulation category, climate regulation is the most representative (32) service, followed by genetic resources (28) from the provisioning category, and from the habitat/support category, the habitat service is the most modelled indicator (18 studies). These top three ESi were mostly identified in research that developed models to estimate ecosystem capacity of carbon storage and sequestration, biomass density, water yield, and raw materials supply. The habitat service is responsible for the maintenance of genetic diversity, and its condition directly affects productivity within the service (McVittie & Hussain, 2013). Cultural ecosystem services (CES) are represented by social-environmental services that support human well-being (Karasov et al., 2020). Within all the studies, the public health service from the cultural category was the least assessed (7). The reviewed studies were organized into ES categories and are presented in the A2. Appendix - Chapter 2, Table A2.2.

2.3.4. Which ML models are implemented?

Among the reviewed studies, 37 implemented classification models to discriminate or delineate ecosystems, 31 modelled ESi through regression, and 12 built both models. All ML models were implemented based on supervised learning (SL), in which the training data are labelled, allowing the improvement of the learner's performance directly. In unsupervised learning (UL) all data are unlabelled, and the machine learns to find structure and new features in the data. UL has the

advantage that does not require training samples, but its accuracy can be lower when compared to SL, which relies on training samples to establish the relationships between inputs and results (Shao & Lunetta, 2012). Figure 2.6a) presents ML algorithms by task (classification and regression) employed more than once in each study.

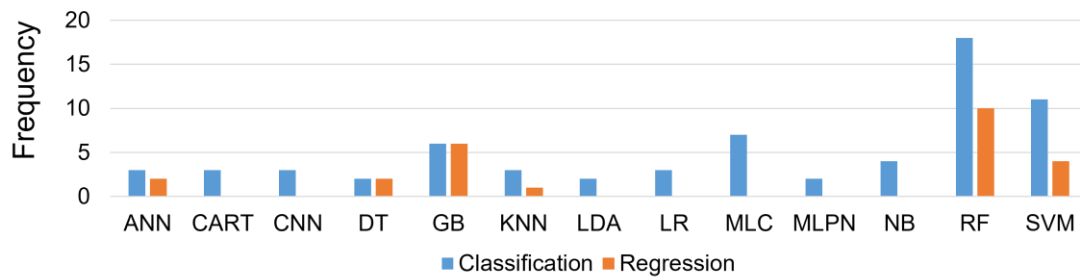
Six studies built two different classification models (Alqadhi et al., 2022c; DeLancey et al., 2019a; Leroux, Falconnier, Diouf, Ndao, Gbodjo, Tall, Balde, Clermont-Dauphin, Bégué, Affholder, & Rounsard, 2020; Matsala et al., 2020; Tarantino et al., 2021; X. Yang et al., 2021a). The most employed algorithms were RF, applied in approximately 50% of the studies, followed by SVM (25%), Gradient Boosting (GB) (20%), Classification and Regression Trees (CART), and Maximum Likelihood (MLC) (more than 10%). Seven studies compared the performance between two to five algorithms (Alqadhi et al., 2022c; Boutsoukis et al., 2019; Fitts et al., 2021; Hunter et al., 2020; Mo et al., 2018; X. Wang et al., 2021; Y. Wang et al., 2017). Five other studies tested more than five learners to compare performance between models (Mouta et al., 2021; Pizarro et al., 2022; Sannigrahi, Chakraborti, et al., 2019b; Sannigrahi, Joshi, et al., 2019; L. Zhang et al., 2022).

Sannigrahi et al. (2019a) and Sannigrahi et al. (2019b) tested 10 ML algorithms to assess ES values and provisioning status based on the classification of ecosystem units. The authors concluded that SVM and RF produced the best classification predictions to assess 9 ESI including spatial proxies of climate regulation, water regulation, soil formation, nutrient cycling, biological control, food production, raw materials, recreation, and cultural services.

Hoffmann et al. (2022) demonstrated in their research the capability of DL to assess the status and functions of habitat and raw materials provisioning services of forest ecosystems. Tarantino et al. (2021) argued that compared to DL algorithms, the SVM classifier was preferred since DL requires larger datasets and more computational resources. Even if it demands higher computational resources, these costs are being overcome with computing power improvements, efficiently allocating computing resources and cloud computing (Mohanty et al., 2020). The authors used proprietary and/or open-source software to build their models and to compute performance comparisons between algorithms and models. Within records, two commercial software were used in ML modelling: See5/C5.0 was used in the classification task and the Cubist (RuleQuest Research, 2022) was used in the regression model. Cilek et al. (2022) classified forest ecosystems and predicted tree cover density as a proxy to estimate carbon storage in coniferous and broadleaf trees, using both software. Google Earth Engine (GEE) (Google, 2023), Weka (Waikato Environment for Knowledge Analysis) (Hall et al., 2008) and biomod2 (Ensemble Platform for Species Distribution Modeling) (Thuiller et al., 2022) were the open-source programs, used to support models' implementation and performance evaluation.

Mouta et al. (2021) employed biomod2 to perform a classification task fusion through eight ML algorithms mapping species' abundance as a proxy of genetic resources service. Boutsoukis et al. (2019) used Weka for modelling habitat service based on estimations of temperate forest canopy height. Around 60% of the studies published after 2019, used the GEE platform as a source of satellite data and/or for imagery and geospatial processing. Open-source platforms and libraries including DL algorithms were also employed by a few studies, such as TensorFlow (Martín Abadi et al., 2015), Keras (Chollet et al., 2015) and scikit-learn (Pedregosa et al., 2011).

a) ML algorithms by task



b) ML algorithms per year

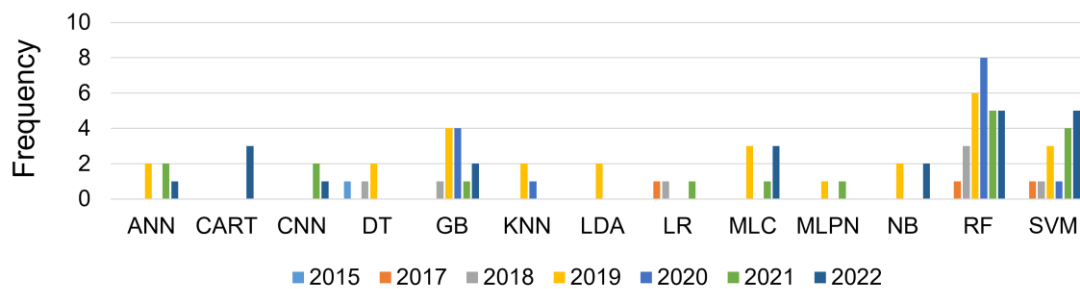


Figure 2.6 - a) ML algorithms used for modelling ES. b) Evolution in the use of ML algorithms through publication years. Legend: ANN - Artificial Neural Networks; CART - Classification and Regression Trees; CNN - Convolutional Neural Networks; DT - Decision Trees; GB - Gradient Boosting; k-NN - k-Nearest Neighbours; LDA - Linear Discriminant Analysis; LR - Logistic Regression; MLC - Maximum Likelihood Classifier; MLPN - Multi-Layer Perceptrons; NB - Naive Bayes; RF - Random Forest; SVM - Support Vector Machines.

Figure 2.6b) depicts the use of ML algorithms through the publication years. Regarding the evolution in ML modelling applications, DT was the first algorithm identified in the literature (2015). In 2017, LR, RF and SVM were the algorithms identified; in 2018 GB was first observed, and RF increased their occurrence; in 2019 were identified modelling applications for all referred algorithms, except for CART, CNN, and LR. This year is coincident with the increased use of GEE for environmental modelling (Arruda et al., 2021; DeLancey et al., 2019a; Fitts et al., 2021; Hoffmann et al., 2022; Hunter et al., 2020; Koskikala et al., 2020; Mallinis et al., 2020; Mpakairi et al., 2022c; Nawrocki et al., 2020; Pipia et al., 2021; Pizarro et al., 2022; Wall et al., 2021; J. Zhang et al., 2019; L. Zhang et al., 2022). Since 2019, there has been an increasing number of publications that performed algorithm comparisons, and hyperparameter tuning as computation power developed, and the use of cloud computing and other platforms and software became more attractive and spread (de Brito et al., 2021). Table A2.3 in the A2. Appendix - Chapter 2 lists all ML algorithms employed by the examined papers.

Hyperparameter tuning was neglected or not reported in 83% of the studies. Selecting appropriate parameters is crucial as improper choices may lead to overfitting or underfitting issues. Table 2.3 summarizes the literature within reviewed studies that have carried out and reported hyperparameters tuning. L. Zhang et al. (2022) conducted hyperparameter tuning to identify the most effective model by comparing validation results across different models with varied hyperparameters. In RF models, the optimal model was determined by testing different numbers of decision trees ($n_{estimators}$). SVM models underwent tuning with various kernel settings and other

hyperparameters to find the optimal SVM model for classification. NB models were compared based on different lambda values. GB models varied in the number of trees for hyperparameter optimization.

Ha et al. (2021) developed an ML model utilizing the CatBoost algorithm, which requires setting up a few hyperparameters, such as depth of trees (depth), number of trees (iterations), learning rate (learning_rate), and L2 leaf regression (l2_leaf_reg) identified as the four most crucial ones. The optimization process employed the GridSearchCV library with five-fold cross-validation. Matsala et al. (2020) and Leroux et al. (2020) tuned GB hyperparameters through a grid search, exploring potential combinations of parameters: shrinkage, interaction depth, number of trees (n.trees), number of observations in the terminal nodes, and bagging fraction. X. Wang et al. (2021) performed a regression task utilizing SVM. The process involved selecting an appropriate kernel function and determining the (c) cost and gamma (g) parameters.

Table 2.3 - ML algorithm hyperparameters tuning.

ML task	ML algorithm and hyperparameter tuning method	Literature
Classification	RF (n_estimators), SVM (kernel), NB (lambda), GB (n_estimators)	L. Zhang et al. (2022)
Classification	CGB (learning_rate, depth, l2_leaf_reg, iterations)	Ha et al. (2021)
Regression	KNN (k), GB (n.trees, interaction.depth, shrinkage, bag.fraction, n.minobsinnode)	Matsala et al. (2020)
Regression	GB (n.trees, interaction.depth, shrinkage, bag.fraction, n.minobsinnode)	Leroux et al. (2020)
Regression	SVM (c, kernel, gamma)	X. Wang et al. (2021)

Spatial analysis and visualization were implemented in Quantum GIS (QGIS) (QGIS Association, 2022), System for Automated Geoscientific Analyses (SAGA), ArcGIS (ESRI, 2023), GEODA1.6.7 (Anselin et al., 2016), FRAGSTATS (McGarigal & Marks, 1995), and an R package, named “spdep: Spatial Dependence: Weighting Schemes, Statistics”, (Bivand et al., 2009). Ten studies employed spatial techniques to evaluate spatial autocorrelation and neighbouring dependency (Han et al., 2022; Hauser et al., 2021; Hoffmann et al., 2022; Mallinis et al., 2020; Mpakairi et al., 2022a; Nzuza et al., 2021; Osborne & Alvares-Sanches, 2019a; Pizarro et al., 2022; Sannigrahi, Joshi, et al., 2019; Y. Zhang et al., 2022). Commonly utilized statistics methods were Spearman and Pearson’s Correlations, Lee’s L statistic, the Global Moran’s I, and the Local Moran’s I indices. These methods were applied to identify spatial autocorrelations, and correlated variables, reduce instability during modelling, mitigate the impact of noisy predictors and redundant data (Nzuza et al., 2021), enhance the efficiency of predictions, and improve the interpretability of final models (Hoffmann et al., 2022).

Applying metrics that do not align with the goals or characteristics of the problem may result in inaccurate evaluations of model performance (Astola et al., 2019). To validate the predictions’ power of the classification tasks, the following metrics were commonly employed: Producer Accuracy (PA) (a total of 14 studies), User Accuracy (UA) (14), Overall Accuracy (OA) (13), and Kappa coefficient (K) (12),

as shown in Fig. 6a). The ROC-AUC (Receiver Operating Characteristic - Area Under the Curve), Precision, and F1-score were used to assess prediction performance also between models in five studies. For imbalanced classification problems, the F1-score was reported to be the best option to measure model quality. Olofsson et al. (2013) do not recommend using just K to assess the accuracy of land use change maps, and Koskikala et al. (2020) evaluated their results with the True Skill Statistic (TSS) arguing that TSS is independent of prevalence, and superior reliability compared to K. The top four classification metrics were UA, PA, OA, and K.

Around 75% of the studies that performed regression tasks used Root Mean Square Error (RMSE) as the primary evaluation metric for assessing the accuracy of predictions (Figure 2.7). The assessment of the agreement between actual and predicted values frequently employed RMSE (24), Mean Absolute Error (MAE) (10), Coefficient of determination (R2) (6), and Relative RMSE (RRMSE) (5). Wang et al. (2017), Mouta et al. (2021), and Hauser et al. (2021) combined RMSE and R2 metrics with Pearson's R and Spearman Correlation to measure correlations between predicted values and observed values. Hauser et al. (2021), and Hoffmann et al. (2022) added Moran's I index to measure the spatial dependence of the residuals' neighbouring points, and Zhu et al. (2022), Pastick et al. (2015), Leroux et al. (2020), and Hudak et al. (2020) measured average model bias through MBE and RMBE.

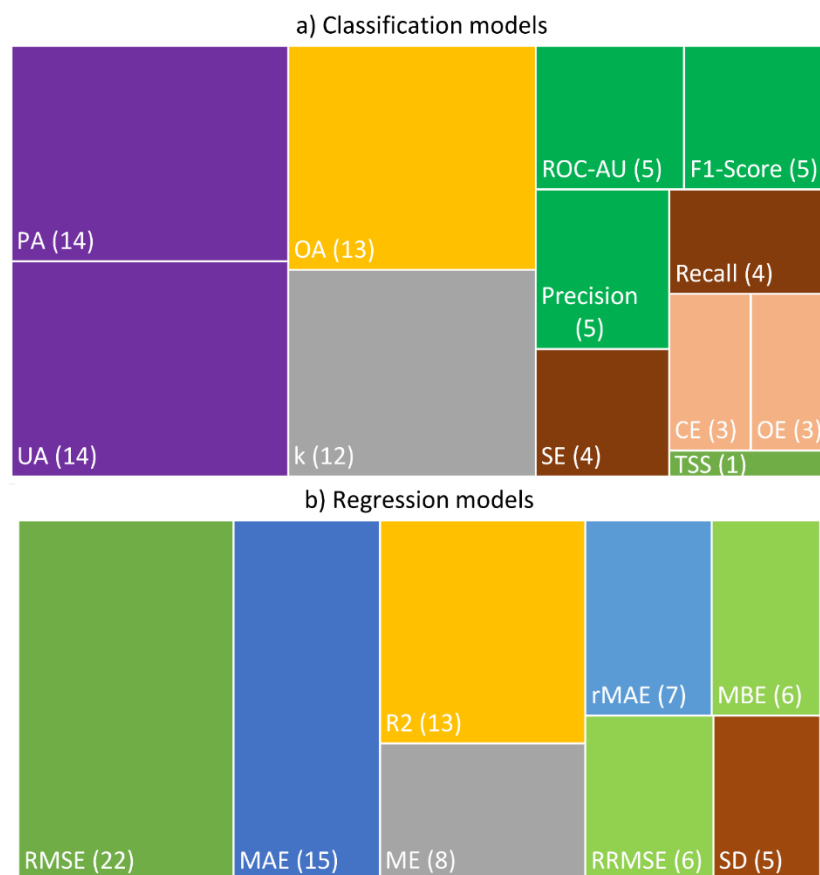


Figure 2.7 - Frequency of evaluation metrics used to assess models' quality. a) Legend (classification models): CE - Commission Error, OE - Omission Error, K - Kappa coefficient, OA - Overall Accuracy, PA - Producer Accuracy, TSS - True Skill Statistics, ROC-AUC - Receiver Operating Characteristic - Area Under the Curve, UA - User accuracy, SE - Sensitivity. b) Legend (regression models): MAE - Mean Absolute Error, MBE - Mean Bias Error, ME - Mean Error, R2 - Coefficient of determination, rMAE -

relative Mean Absolute Error, RMSE - Root Mean Square Error, RRMSE - Relative RMSE, SD - Standard Deviation. The number in parenthesis refers to the number of studies

2.3.5. What is the relationship between ML tasks and ESi?

The plot in Figure 2.8 relates ESi with ML tasks, highlighting their correspondence. The classification was the most performed task within ES categories, habitat/supporting (21), regulating (19), provisioning (13), and cultural (4), against seven, nine, five, and one, respectively, for regression tasks.

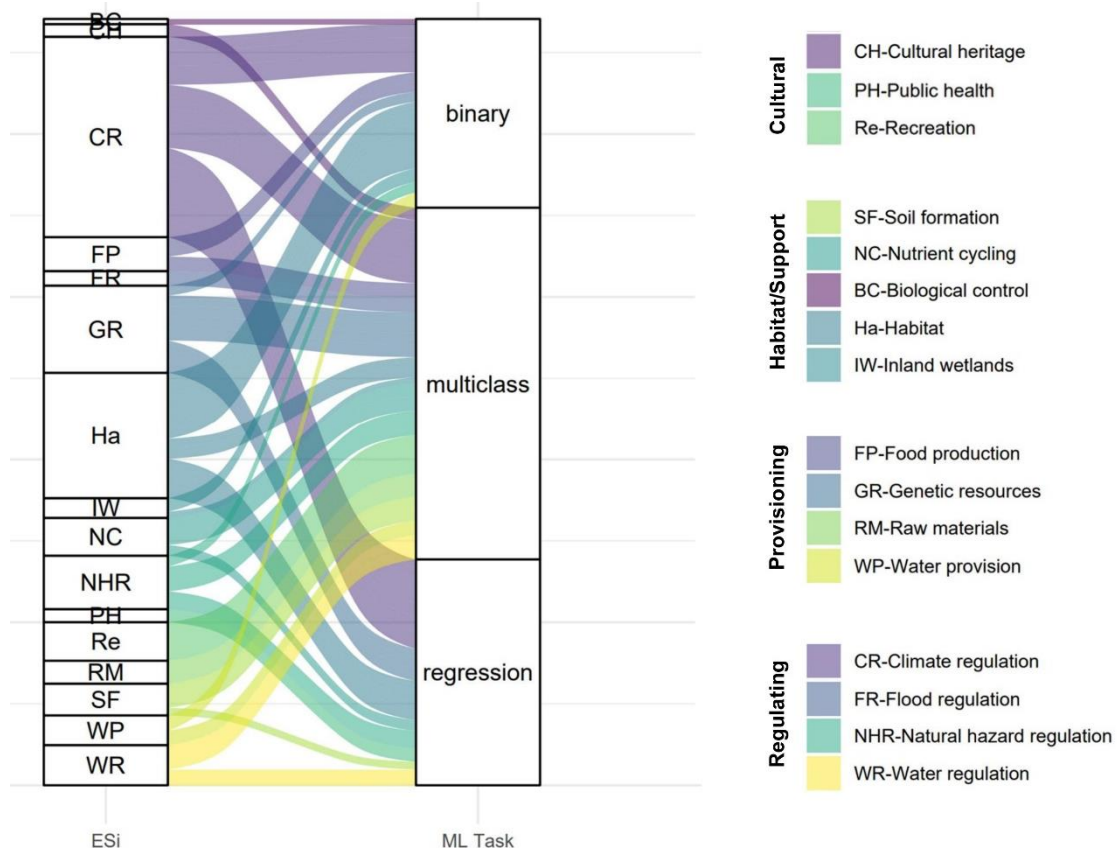


Figure 2.8 - Correspondence plot relating ML tasks within ES indicators (ESi).

Among classification tasks, 44% of studies were multiclass problems and 28% were binary classifications employed to create presence/absence maps. Binary classifications were mostly implemented in studies assessing habitat (10) and climate regulation (4). In a multiclass scenario where many values are discriminated into many classes, climate regulation (7), genetic resources (5), and habitat (4) were the most modelled indicators within studies. The classification tasks performed for taxonomic mapping or habitat discrimination were done in two steps. First, a map delineating the ecosystem was created, and then its output was used as a mask to discriminate species and habitats. Tarantino et al. (2021) first extracted the grassland layer by performing binary classification and then used this as an input for the second step, which was a multiclass problem to classify four grassland habitats. Matsala et al. (2020) first predicted land cover classes to produce a forest cover mask and then used the predicted map to classify dominant tree species.

Predicting continuous values through regression tasks was mostly performed by climate regulation (7), genetic resources (5), and habitat (4) indicators. Nearly 55% of studies that performed a regression task predicted carbon storage in forests, woodlands, grasslands, croplands, and tundra ecosystems, as a proxy of climate regulation services. Other representative dependent variables were tree cover density, leaf area index, and leaf mass area, estimated as spatial proxies for timber production within raw materials provisioning services, as well as modelling crop production as a proxy for food provisioning, and the prediction of dissolved inorganic nitrogen (DIN) and reactive phosphate (PO₄-P) levels, to assess nutrient cycling, water quality regulation, and water provision services.

2.3.6. Is there a rule for model development within ESi?

Approximately 24% of the studies built their models by applying both, classification, and regression tasks (Table A2.4, A2.Appendix - Chapter 2). Classification tasks were mostly employed to create land cover maps or discriminate ecosystems as the first step of nearly a quarter of the developed ML models. These maps sometimes combined with other variables were used as input for further regression models.

Meta-analysis was carried out by grouping reviewed studies within the 16 ESi identified. We found that 69% of estimates had negative log response ratios (log [RR]), varying from -0.92 to 0.41. With a 95% confidence interval (CI) (-0.80 to -0.05), the estimated average log [RR] based on the random-effects model was $\mu=-0.42$. As a result, the average outcome differed significantly from zero ($z=-2.2194$, $p=0.0265$), and the Q-test supports the hypothesis that the outcomes were not statistically heterogeneous ($Q=2.0623$, $p=1.0000$, $\tau^2=0.0000$, $I^2=0.0000\%$). A forest plot with the estimated results grouped by indicators and based on the random-effects model is depicted in Figure 2.9.

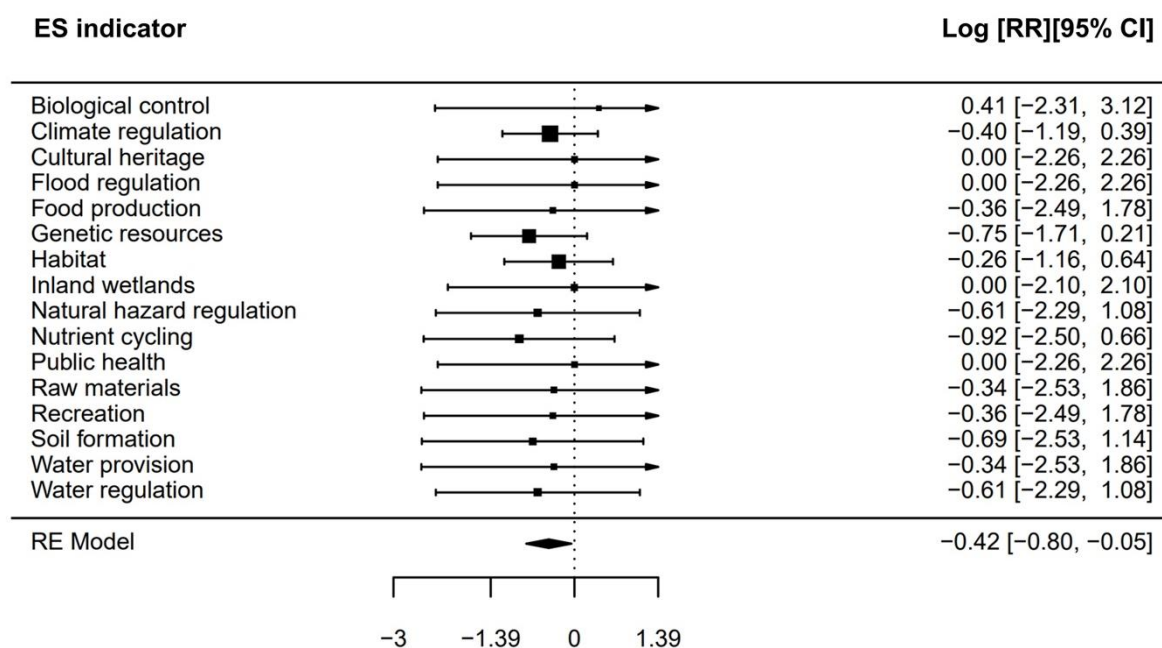


Figure 2.9 - Forest plot with the log [RR] estimates using 95% of CI.

Results indicate that, on average, there is a 65% likelihood of utilizing classification and regression for assessing ESi. Biological control, cultural heritage, flood regulation, food production, inland wetlands, public health, raw materials, recreation, and water provision, were the indicators likely not to employ a classification as a first step in the models. On the other hand, studies assessing climate regulation, genetic resources, habitat, natural hazard regulation, nutrient cycling, soil formation, and water regulation were all investigated employing both tasks.

Analyzing the percentage of weights given to each indicator during the model fitting evidence indicators influence (Figure 2.10a). Climate regulation (2), genetic resources (6), and habitat (7) had a relatively high weight compared to the other indicators, being influential indicators, but not outliers. The radial graph evaluates the consistency of the results considering standard errors and variances of samples (Figure 2.10b). The value of the log [RR] is represented by the line projected from (0,0) through the corresponding value in the arc (-0.42). The graph indicates good consistency of results clustering the three influential indicators (climate regulation, genetic resources, and habitat).

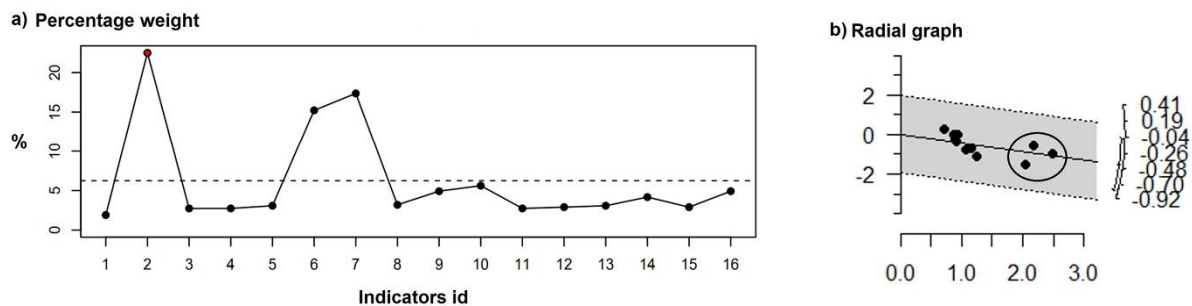


Figure 2.10 - a) Percentage weights plot for the 16 ESI examining the use of classification tasks in regression models. b) Radial graph. Legend Indicators id: 1 - Biological control, 2 - Climate regulation, 3 - Cultural heritage, 4 - Flood regulation, 5 - Food production, 6 - Genetic resources, 7 - Habitat, 8 - Inland wetlands, 9 - Natural hazard regulation, 10 - Nutrient cycling, 11 - Public health, 12 - Raw materials, 13 - Recreation, 14 - Soil formation, 15 - Water provision, 16 - Water regulation. Radial graph of the model fitted.

2.4. DISCUSSION

In this systematic literature review, we explore the development of ML models for assessing ES based on RS data from Sentinel-2 and Landsat satellites. The review sheds light on the most frequently assessed ES, prevalent algorithms, tasks, and evaluation metrics applied in satellite-based ML modelling. The evolving integration of ML into ES modelling demands a deeper understanding of the models' implementation and development, their applications across various ES, and the identification of avenues for future research.

2.4.1. Summary of results

Modelling spatial proxies of ES based on high spatial and spectral resolution satellites enables a more consistent characterization of ESI components that are essential to sustainably managing natural

resources (Guirado et al., 2019). It facilitates rapid, frequent, and continuous observations, thereby enhancing monitoring capabilities (del Río-Mena et al., 2023).

High spatial resolution sensors capture more detailed and accurate information about an object when compared to medium spatial resolution satellites (Liang & Wang, 2019). Multispectral sensors can detect small differences in spectral signatures, as they have contiguous bands with small bandwidths (<20 nm), consequently, producing more accurate classifications (Hunter et al., 2020). Nevertheless, the utility of optical sensors is constrained by limitations such as daytime image acquisition and vulnerability to cloud cover, atmospheric haze, or dense vegetation canopies (X. Wang et al., 2021).

Data fusion integrating observations from different instruments provides advanced knowledge of the relationship between landscape dynamics, ESI, and human activities (Ramirez-Reyes et al., 2019). The approach is becoming more frequent in ES-related research and was employed in 53% of the reviewed studies, including integration of Sentinel-2 and/or any Landsat missions with Sentinel-1, Rapid Eye, MODIS, World View-2, IceSat-2, Planet Scope, SPOT-6, and manned and unmanned aerial vehicles. This observation agreed with Schirpke et al. (2023), emphasizing the increased adoption of the data fusion approach, as well as the inclusion of a wide variety of ancillary data, such as climatic and topographic variables, population density, census data, road networks, number of trees, soil type, and geology. Vylvlečka and Pechanec (2023) demonstrated in their review a preference for Sentinel-2 over Landsat 8, with spatial and spectral resolutions being a crucial factor affecting accuracy. Our results are also aligned with these statements, and some reviewed papers clearly state that (Koskikala et al., 2020; Lobert et al., 2021; N. Pastick et al., 2018).

A total of 16 ESI were identified (i.e., biological control, climate regulation, cultural heritage, flood regulation, food production, genetic resources, habitat, inland wetlands, natural hazard regulation, nutrient cycling, public health, raw materials, recreation, soil formation, water provision, and water regulation). These indicators derived from satellite-based ML modelling, enable the assessment of ecosystem structure, configuration, and patterns of changes that influence nature's ability to provide goods and services (Olander et al., 2018).

The identified ESI aid in informed decision-making through extrapolating measurements of ecosystems' extent and conditions. These outcomes provide valuable support for landscape planning and management through physical measurements, enabling tracking changes in ecosystem assets, species distribution, and ecosystem health (King et al., 2024). When integrated into socio-economic data, ESI can contribute to the design of ecosystem accounting, providing information on natural stocks and aiding in the development of national accounts and public policies, enabling better-informed and sustainable management practices (Fleming et al., 2022). Nevertheless, ecosystem monetary accounting and monitoring still require direct measurements, and ESI would not be enough.

Within the reviewed studies, only 10% evaluated monetary accounts of ES calculating the benefits generated by each service or category of services (Alqadhi et al., 2022c; Han et al., 2022; Kundu et al., 2022; Mugiraneza et al., 2019; Sannigrahi, Chakraborti, et al., 2019b; Sannigrahi, Joshi, et al., 2019).

Approximately, 80% of studies assessed 20% of the ESI identified. The ESI categories with the most frequently developed ML models and applications were regulating (with climate regulation), provisioning (with the provision of genetic resources and raw materials), and habitat (with habitat service providing maintenance of genetic diversity). The condition of the habitat providing the service

directly affects the availability of many other ecosystem functions and services (McVittie & Hussain, 2013). Natural habitats are crucial to maintaining genetic resources, and biodiversity (Reddy, 2021). Mapping tree-species distribution, canopy height, and tree cover density allowed for measuring the ability functions of climate regulating services such as carbon storage and sequestration, and raw materials provisioning, such as timber, biomass, and other tree-derived products (Hudak et al., 2020).

ML serves as a powerful complement to current methods rather than a substitute (Scowen et al., 2021). Assessing ESI using ML models is a good decision when one follows a set of good practices and has well conceptualized the study's purposes (Willcock et al., 2018). When one chooses an algorithm just because it is trending or easier to implement, it is quite dangerous, because it can be effective in solving certain problems, but not for a specific problem and/or dataset (Craven et al., 2023). A good practice is to test performances between models and learners and monitor the results through a wide range of evaluation metrics (Domingos, 2012).

ML tasks are demanding in terms of computing, particularly when modelling big earth data (Ma et al., 2019). Nowadays, there is a wide variety of algorithms, and most of them do not have many requirements to implement, unlikely most of them are highly sensitive to the quality of the training data, as well as to hyperparameter configurations (Maxwell et al., 2018). Inevitably, before building ML models, it is essential to understand the algorithms' drawbacks and limitations, such as lack of transparency, hyperparameter sensitivity, generalizability through overfitting and underfitting, power computing needed and time-consuming (Scowen et al., 2021).

Biases, inaccuracies, or missing data can significantly impact model performance, as ML models require sufficiently large, representative, and diverse data to capture the underlying patterns, and generalize well to new, unseen instances (Bishop, 2006). The low accuracy of models often stems from inadequate training data, regarding insufficient quantity and quality, and imbalances in the distribution of classes or features (Hastie et al., 2009). To improve the robustness and reliability of ML models, data preprocessing, cleaning, augmentation, and oversampling techniques lead to better accuracy and more trustworthy results (Craven et al., 2023).

A lack of transparency can be a significant barrier to understanding how the model arrives at its predictions and contributes to the *black box* problem, making it challenging to decipher the reasoning behind the results (Schirpke et al., 2023). Nonetheless, learners can be transparent and repeatable, and algorithm development is calling for advances that better link inputs, outputs, and intermediary steps (Nikparvar & Thill, 2021).

RF was the most implemented algorithm, followed by SVM. The advantages of using RF instead of CART are the robustness to overfitting and the predictors' value range aggregation (Breiman, 1984). The number of hyperparameters required by the RF classifier is less than the number required for SVM and other algorithms (Boser et al., 1992). In contrast to many algorithms, including SVM, RF might face challenges when dealing with imbalanced data. On the other hand, SVM tends to perform better under such circumstances, thanks to its generalization capability, overall robustness, high accuracy, and suitability for situations involving limited training data (Pizarro et al., 2022). Choosing an algorithm that fulfils the requirements of each model is quite challenging. Making use of tools that compare algorithms and models is a better option, as they also commonly offer various elements of data handling, processing, and performance evaluation.

The primary result of the meta-analysis was to assess the overall feasibility of using hybrid models, which involve completing both classification and regression tasks. Measuring the effects of implementing hybrid models instead of a single application provides a better understanding of researchers' decisions and the applicability of combining tasks in the assessment of ESI.

Classification tasks were mostly employed to identify and delineate ecosystem assets, such as forests, and estimate their extent, while regression tasks were modelled to evaluate ecosystem conditions by predicting specific characteristics (e.g. tree cover density). Besides, some studies implemented a two-step modelling strategy, integrating both classification and regression tasks. This synergistic method allows for a comprehensive and optimized use and analysis of satellite-based ML techniques to assess ESI, as well as contributes to more robust and accurate modelling outcomes in ES assessments.

2.4.2. Common challenges and opportunities

Many studies highlighted opportunities for leveraging SEO in ESI assessments and stressed the need for addressing challenges through innovative funding and partnerships to enhance global ES assessments (Lobert et al., 2021). Challenges related to variable and model accuracy, data accessibility, technology availability, and ethical considerations were pointed out as topics that require attention to ensure inclusive and meaningful technology use (Narine et al., 2019). Few records suggest that integrating different technologies, fostering transdisciplinary collaboration, and exploring advancements in related research fields could provide further insights into ES research (Alqadhi et al., 2022c; Kundu et al., 2022; Mpakairi et al., 2022a; Vidal-Macua et al., 2020a).

Limitations have been overcome through methodological and technical advancements in cloud computing, efficient resource allocation, algorithm improvements, and quantum information technologies (European Spatial Agency, 2023; Willcock et al., 2023). These developments have been fast-evolving and fostered by institutions and agencies, such as NASA, USGS, and ESA (Vývlečka & Pechanec, 2023), as well as, satellite data streams, e.g. GEE and the Open Data Cube (ODC, 2018), facilitating access, management, and analysis of SEO data. Coupled with advances in open-source data science algorithms and packages, cloud-based technologies are facilitating the modelling workflow for a broad spectrum of ecosystem functions and services (DeLancey et al., 2019a). Furthermore, fostering the applicability of such models and technologies in landscape planning, governance, and policymaking (King et al., 2024).

The rapid technological evolution in RS is calling for the development of approaches and techniques that can be used on SEO-based monitoring strategies of ESI. However, fieldwork remains crucial for some ES assessments, as RS is not a substitute for field surveys, ground-based sensors and sensor networks, and measurements derived from SEO may need to be validated through field observations (Jullian et al., 2021). The constraints imposed by the available ground-based datasets were one of the main limitations reported in the studies. Matsala et al. (2020) stated the need for a national statistical inventory in Ukraine, as a barrier met in implementing their research. M. Zhang et al. (2019) pointed out that the temporal misalignment between SEO and field survey data caused by the absence of cloud-free Landsat scenes that precisely match ground observation times introduces errors in result estimations. Sharma et al. (2018) emphasized the crucial role of extensive ground data in calibrating and validating classification outputs and the need for a robust methodology capable of accurately quantifying crop production at the field scale. Therefore, integrating ground sensor data helps validate

the quantification of ecosystem functions, complementing the central role of satellite data (Vývlečka & Pechanec, 2023).

Achieving accurate predictions of ESI from remotely sensed data requires a profound understanding of the intricate relationship between spectral information and each proxy (Ørka et al., 2022). This task is particularly challenging due to the unobservability, or measurement difficulties associated with many ES (del Río-Mena et al., 2023). Furthermore, adapting locally derived ES models to new locations or different scales faces limitations due to the need for parameterization, calibration, and validation, often impeded by the absence of ground truth data (Cord et al., 2017).

Leveraging a diverse range of SEO instruments and measurements, suitable datasets can be chosen or developed for estimating specific ESI. This approach is expected to accelerate progress in spatially characterizing ESI, thereby contributing to ecological conservation, management, and integrated land-use planning (Andrew et al., 2014).

Despite the growing application of ML in ESI modelling, a substantial number of studies lack a dedicated focus on research commitments to ensure the replicability of methods and reproducibility of existent datasets. To address this gap, an easily understandable and transparent framework capable of reliably modelling unstructured data, such as images, video, time-series data, and text is required. As these diverse data types are increasingly integrated into ESI modelling throughout data fusion approaches, effectively handling and reproducing them may need domain expertise and the application of reverse engineering techniques.

The development of automated functions, akin to those found in ML Operations (MLOps) (Kreuzberger et al., 2023), is essential to streamline the process of taking ML models to production and subsequently maintaining and monitoring them in the context of satellite-based ESI modelling (Urbanowicz et al., 2022a). These automated functions play a key role in optimizing modelling performance, capturing complex associations in data, enhancing interpretability and reproducibility, and preventing and detecting common sources of errors throughout the model's life cycle (Poleshchuk et al., 2022).

To ensure the robustness of the chosen model, resampling techniques must be employed for model tuning and predictor selection (Guio Blanco et al., 2018). Accordingly, there is a growing need for wider reporting of the specific tuning, predictor selection, and resampling methods utilized, given their substantial impact on prediction uncertainty and the identification of crucial predictor variables.

The ongoing advancements in cloud computing, open-access data, and ML technologies are expected to propel the development of large-scale ecosystem inventories (DeLancey et al., 2019a). These advancements will not only expand the user base for geospatial data but also foster collaboration, addressing both existing and emerging challenges in large-area mapping and monitoring.

Developing models that can be scalable and replicable must consider uncertainties related to each phenomenon and spatial scale and a well-developed proof of concept of its applicability (Kubiszewski et al., 2022). Therefore, the scalability of models is achievable due to their rapid and cost-effective development (Scowen et al., 2021). The utilization of open-source tools and models plays a crucial role in fostering the widespread adoption of ML techniques, particularly for high-dimensional and multi-modal data. Additionally, the automation of data analysis is a key requirement underlying the efficiency and effectiveness of these models (Nikparvar & Thill, 2021).

2.4.3. Research limitations, contributions, and directions for future studies

Synthesizing the review of the included studies through meta-analysis helped in building knowledge of the SEO data-based ML applications. However, biases can lead to underestimations or overestimations in any review conclusions (Sterne & Egger, 2005). Many types of systematic errors might affect a review, but selection biases are the internal biases more frequently recognized as causes of reviews' conclusions deviations (Nakagawa et al., 2022). The selection bias occurs when the selected studies represent a small population of all research, and the absence of specific studies could increase biases (Greco et al., 2013). We are aware of the consequences of limiting the research to the English language, as this excludes worldwide outstanding studies reported for example in Chinese, Spanish or Portuguese. Some biases can also exist due to our decision to focus the review on studies that employed Landsat (4, 5, 7 and 8) and/or Sentinel-2A/2B. We also acknowledge that many other studies not included in this review would develop ML models to assess ESI using data from Sentinel-1A/2B, MODIS, Lidar, or other RS technologies; as well as other studies that model ESI, but did not choose to use "ecosystem services" in their title, keywords, and abstract. The methodology implemented allows users to assess, replicate, or update the review's findings. These results contribute to a better understanding of the use of SEO data and technologies, and the applicability of ML models to assess ESI.

As the assessment and monitoring of changes in ESI are helping decision-makers to achieve sustainable development and management at multiscale (Guirado et al., 2019), the outcomes of this review are relevant information for society and the scientific community, highlighting the latest approaches that significant researchers have produced worldwide.

Meta-analysis built the evidence that even when a problem is to predict continuous values, a classification task is commonly taken first, confirming ES-related researchers' adherence to ML techniques. Studies applied hybrid models when there were no available data identifying and delineating the target ecosystem, and further implemented a regression task to estimate ESI.

In future studies, ES researchers may adopt standardized methods to present the intricate steps related to data collection and processing, analysis, visualization, and interpretation of results, as suggested by Scowen et al. (2021). But for that, a conceptual framework that guides model replicability needs to be developed and disseminated through the scientific community and stakeholders to enhance the applicability and understanding of ESI modelling. Additionally, future research may provide the required background to advance beyond what can be done and what can yet be enhanced when applying ML to estimate ES conditions. As this study did not analyze the predictors used in the various models, this is one of the topics that needs further knowledge and discussion, addressing this and other gaps including reviewing the use of spectral indices, and other landscape metrics as predictors, and handling the increasing volume of data developing tools that lower the costs associated with ES modelling.

2.5. CONCLUSION

The purpose of this systematic review was to summarize studies that developed satellite-based ML models to assess ESI and analyze their relationship, adopting a methodology that enables users to evaluate, repeat or revise the review's findings. Results show that there are no rules regarding the selection of ML tasks, algorithms, or evaluation metrics, but meta-analysis indicates the likelihood of

applying classification and regression tasks, specifically when assessing climate regulation, habitat, and genetic resources. ML models based on SEO data are a promising method to assess ESi, with increased potential if combined with ground truth data of monitoring campaigns. Advances in automated methods for ES valuation are cost-effective and allow for better management of natural capital. However, further effort is needed to establish a robust and user-friendly framework for ML applications in ES modelling, ensuring not only the reliability of results but also facilitating the integration of diverse data sources and the deployment of models into operational settings. This includes the development of automated processes, inspired by MLOps, to efficiently manage the lifecycle of ML models within satellite-based ES applications. The main subjects of the reviewed studies related to environment protection, ES assessment and evaluation, nature conservation, natural capital management, policymaking, and land use and landscape planning. Modelling climate regulation services, such as carbon storage and sequestration, remained the overarching goal of 30% out from the reviewed studies. Additionally, measurements of nature stocks, such as biomass, freshwater, food production, and raw materials, have shown to be important at a global scale. The outcomes of this review add value to the present state-of-the-art on the applicability of ML models to assess ES through ESi. It further identifies the most relevant techniques and applications that support environmental problems.

STAGE 2: PROOF OF CONCEPT

Satellite-based ML modelling has emerged as a powerful tool to understand and quantify spatial relationships between ES and human well-being. As SEO technologies continue to advance, there is an increasing opportunity to harness ML techniques to better assess ES. The research findings of stage 1 illustrated the utilization of ML models in evaluating ES and underscored the connections between established methods and their applicability and replication. Additionally, it presented current perspectives on existing satellite-based approaches and argued that there were no specific rules regarding the selection of ML tasks, algorithms, or evaluation metrics. It also pointed out the need to advance data and algorithms fusion integration approaches, and to establish a robust and user-friendly framework for Satellite-based ML applications in ES modelling, ensuring not only the reliability of results and the integration of diverse data sources but also the deployment of models into operational settings.

In this scope this stage aimed to demonstrate the feasibility, robustness, and replicability of research, providing proof of concepts and testing data and algorithms in strategic areas before implementing them at the national scale. The main outputs are modelling different spatial and temporal scales, and testing data and methods, providing guidelines to basis the development and implementation of research at the country level. This stage includes two published scientific productions presented in chapters 3 and 4. The study depicted in Chapter 3 focused on applying sensitivity analyses to test and find the best predictors for modelling freshwater ecosystems, building a framework of global geospatial data, and presenting application baselines to support estimating WWPI in different spatial and temporal scales. Chapter 4 presents a study based on a common concern about advancing the knowledge of methodologies, tools and strategies to improve the development of satellite-based data-driven models of GBE. This study proposed a two-step modelling strategy that helps to manage and analyze effectively large geospatial datasets while enhancing overall efficiency in GBE mapping workflows, combining techniques to take advantage of different methods by developing a hybrid modelling approach to classify GBE and estimate their relationship considering seasonality.

Chapter 3: Almeida, B., & Cabral, P. (2023). Data-Driven Modelling of Freshwater Ecosystems: A Multiscale Framework Based on Global Geospatial Data. In C. Grueau, A. Rodrigues, & L. Ragia (Eds.), International Conference on Geographical Information Systems Theory, Applications and Management: GISTAM 2023 (Vol. 1, pp. 104-111). <https://doi.org/10.5220/0012037800003473>

Chapter 4: Almeida, B., & Cabral, P. (2024). A hybrid modelling approach for detecting seasonal variations in inland green-blue ecosystems. *Remote Sensing Applications: Society and Environment*, 33, 1-15. Article 101121. Advanced online publication. doi.org/10.1016/j.rsase.2023.101121

3. DATA-DRIVEN MODELLING OF FRESHWATER ECOSYSTEMS: A MULTISCALE FRAMEWORK BASED ON GLOBAL GEOSPATIAL DATA

3.1. INTRODUCTION

Anthropogenic and environmental factors threaten the existence of natural ecosystems that depend directly or indirectly on the presence of water in a landscape (Mpakairi et al., 2022d). Those ecosystems are biodiversity hotspots that require access to water to maintain the communities of plants and animals, the ecological processes they support, and the services they provide (Shi et al., 2014). In dry periods, there is less water in rivers, and over-exploitation depletes the natural water table and affects these vulnerable ecosystems (Sharma et al., 2018).

The status of water resources degradation and scarcity gets worse as human activities directly cause an increase in the local drying initiated by climate (Kløve et al., 2014). Adverse atmospheric conditions impact water resource availability, compounding the challenge of integrated water management, concerning quality, quantity, and ecosystem support (Novo et al., 2018). In the face of climate change and ever-more intensive land use, conceptual models, and quantitative assessments of surface and groundwater interactions with the environment are needed (X. Yang et al., 2021a).

The increasing global demand for water for agriculture, domestic, and industrial needs, requires integrated management of natural resources (Almeida & Cabral, 2021). Therefore, there is a lack of knowledge on the existence of conceptual frameworks and guidelines useful to model freshwater ecosystems (Cui et al., 2021). The process of acquiring geospatial data is the most challenging part of environmental modelling (Meddens et al., 2022). Frameworks to support data-driven modelling must incorporate the knowledge that facilitates spatial and spatiotemporal data acquisition and baselines that guide conceptualization and model implementation (Nti et al., 2022).

When there are few or no guidelines for sources of geospatial data and their environmental applications, searching and applying exhaustively all the possibilities is not a feasible option. Even with very sophisticated computers, the running time needed would be unacceptable, or could not add any value for the model in terms of quality. Several studies have been developing methodologies for modelling water ecosystems using remote sensing and machine learning, such as Kundu et al. (2022) detecting water richness change, Mpakairi et al. (2022) assessing spatiotemporal variation of vegetation heterogeneity in groundwater-dependent ecosystems, and Sharma et al. (2018) estimating impacts on the water resources from crop irrigation. In synthesis, we observe that some of the previously proposed approaches solve the problem very well, but none of them was presenting possible sources of global spatial data and performed a sensibility analysis of their use and applications in modelling water ecosystems.

The Copernicus Land Monitoring Services (CLMS) provides the basis for integrated analysis of the main drivers of land use change to inform about Europe's natural resources and their status (Copernicus Programme, 2023). It offers information services based on satellite Earth observation freely and openly accessible to its users, only requiring registration and referencing. In the portfolio of the High-Resolution Layers (HRL) under the *Experts and National Products archive*, exist five thematic layers on land cover characteristics at 10m spatial resolution, covering 39 European countries. The HRL Water and Wetness (WAW) 2018 datasets are based on imagery covering the period 2012-2018. They were

created based on satellite imagery, including ESA's Sentinel-1 and Sentinel-2 satellites and spectral indices such as the Normalised Difference Water Index (NDWI) and its modified version mNDWI, as well as the Normalised Difference Vegetation Index (NDVI).

The goal of this study is to present a set of reference data and application guidelines that support reproducing the WWPI with quality. For that, we developed machine learning (ML) models and performed sensitivity analyses to find the best predictors. The ML models were implemented in a transnational river basin district (Portugal – Spain), the Tagus Basin. Satellite imagery, satellite-derived data, biophysical variables, and landscape characteristics were the explanatory variables evaluated in the sensitivity analyses.

The framework comprises a set of global open-access data, that can be used to model freshwater ecosystems at multiscale (spatial and spatiotemporal). The outcomes of this research would increase our understanding of the use and replicability of the Copernicus data, and knowledge in implementing data-driven models based on SEO data in different years and locations. The developed framework comprises a set of baselines for predicting the spatial distribution of water and wetness status and conditions allowing the assessment of the impacts of drivers of changes on freshwater ecosystems.

3.2. MATERIALS AND METHODS

3.2.1. Study area

The Tagus Basin in Portugal is the most important source of water in the country due to its productivity, and quality of water (Ribeiro, 1998). The river basin resources are responsible for economic and demographic expansion through the years (Mendonça, 1990).

The extensive network drainage promotes easy access to water and supports the development of intensive agriculture (Almeida, 2020), such as annually harvested plants including flooded crops such as rice fields and other inundated croplands, and permanent crops such as vineyards, fruit trees and olive groves (Novo et al., 2018). Forest and seminatural areas are represented by mixed forest and transitional woodland/shrub (Ramos et al., 2017).

Due to its strategic location in the surroundings of Lisbon, the most populated region of the country, there is a growing need for changes in land use to develop artificial surfaces such as urban fabric, road and rail networks, airports, dump sites and industrial areas (Mendes et al., 2015), which is compromising water resources and dependent ecosystems in the basin.

3.2.2. Data

3.2.2.1. Dependent variable

The necessary data to implement a learning machine process is commonly divided into training, validation, and test datasets (Domingos, 2012). The training data are the predictors, the validation dataset is used to control the learning process and the test dataset is employed to assess the learner's performance. To predict continuous values such as the Water and Wetness Probability Index (WWPI),

regression tasks were carried out. The target in the regression models is the response variable, also known as dependent variable.

The WWPI is a raster displaying the occurrence of water and wet areas as an index on a scale between 0 (only dry observations) to 100 (only water observations) (Copernicus Programme, 2023). It indicates the degree of wetness in a physical sense, independently of the actual vegetation cover. The landscape elements included in the datasets are permanent and temporary open water bodies, temporarily inundated areas, wet agricultural fields, and transitional coastal water bodies (European Environment Agency, 2023).

3.2.2.2. Explanatory variables

The main goal of this study is to find the best predictors to enable an accurate reproducibility of the WWPI dataset. A wide variety of data such as satellite imagery, satellite-derived data, biophysical variables, and landscape characteristics, were evaluated through sensitivity analysis.

Single bands from Sentinel-2 images and satellite-derived indices were the first predictors evaluated in the sensitivity analysis. This satellite has a high-resolution multispectral sensor acquiring and recording information in 13 bands: visible (VIS with 4 bands), near-infrared (NIR with 6 bands) and shortwave infrared (SWIR with 3 bands). This instrument can detect small differences in spectral signatures, as they have contiguous bands with small bandwidths (<20 nm), and consequently acquire more accurate information (Hunter et al., 2020). The Sentinel-2 mission is providing data from 2015 until 2025 with a temporal resolution of 5 days, and spatial resolution of 10, 20 and 60m.

The combination of algebraic operations in pre-established bands leads to the definition of indices that allow highlighting certain information (i.e., water, vegetation, soil, minerals, etc.). Spectral-derived indices result from combinations of two or more spectral bands designed for the enhancement of specific objects (Kuenzer et al., 2014). NDVI, NDWI and Normalized Difference Moisture Index (NDMI) were calculated and included as predictors.

Climate variables, such as precipitation and evapotranspiration combined with topography are important drivers in water modelling (Ringersma et al., 2003). The annual precipitation was obtained from the WorldClim database (Fick & Hijmans, 2017) and the Global Potential Evapotranspiration (Global-PET) and the Global Aridity Index (Global- Aridity) from the Consortium of Spatial Information, Global-Aridity and Global-PET Database (Trabucco & Zomer, 2019). Global data precipitation was obtained from spatial interpolation of nearly 60 000 weather stations providing monthly climate data. The datasets have a spatial resolution of approximately 1 km². Reference evapotranspiration and global aridity were derived from the WorldClim precipitation model and have the same spatial resolution and temporal scale.

Topographic data are globally available from NASA through the Shuttle Radar Topography Mission (SRTM). The dataset was released in the year 2000 with approximately 30m pixel resolution.

Table 3.1 lists the datasets used to estimate WWPI, specifying the source of data and the pixel resolution.

Table 3.1 - Description of the datasets, their source and pixel resolution.

Data	Source	Pixel resolution	Subject	Scale
Satellite Data	Copernicus Open Access Hub (https://browser.dataspace.copernicus.eu/)	10m	-	Global
Digital Elevation Model (DEM) (m) & Slope (SLOPE) (%)	NASA Shuttle Radar Topography Mission (https://www.earthdata.nasa.gov/)	30m	Topographic	Global
Average Annual Precipitation (mm)	WorldClim (https://worldclim.org/)	1km	Climatic	Global
Global Potential Evapotranspiration (Global-PET) (mm)	Consortium of Spatial Information-CSI (http://www.cgiar-csi.org)	1km	Climatic	Global
Global Aridity Index (Global-Aridity)	Consortium of Spatial Information-CSI (http://www.cgiar-csi.org)	1km	Climatic	Global

3.2.3. Model Design

In regression problems, the target values are continuous, and the machine consistently improves learning to better fit the model. The expected output was a predictive spatial model implemented in geographic information systems using ArcGIS Pro 2.9.0 software (ESRI, 2023). The task was to build a regression model using a non-parametric approach that enables the replicability of the WWPI with quality. The relationship between explanatory variables and the response variable was modelled through the tool *Train Random Trees Regression Model*.

The Random Trees algorithm is an adaptation of the Decision trees (DT) (Breiman, 1984) in a GIS environment. It is a nonparametric approach that iteratively divides a dataset into increasingly smaller subgroups using the same splitting decision (J. Zhang et al., 2019). The decisions are made according to the rank order of importance, optimized by a randomized procedure (Mallinis et al., 2020). DT can inherently handle nonlinear relationships, mixed predictor categories, and data gaps, and is resistant to outliers and the effects of collinearity (Osborne & Alvares-Sanches, 2019a). The disadvantage of the DT is related to the models' fitness and instability due to the propagation of errors down through subsequent splits in the tree (Breiman, 2001).

The input datasets comprising the explanatory variables and the target were in raster data format. As the cell size affects the training result and the processing time, this parameter was set up in the environment settings to make sure that the training process will keep the pixel size of 10m, as same as the target. The *Percent Samples for Testing* were set to 20%, meaning that one-fifth of the training sample was used to measure the error for interpolation in space, called test location points. This

parameter evaluates three types of errors: errors on training points, errors on test points, and errors on test location points. The maximum number of trees, the maximum tree depth and the maximum number of samples were set by default with values of 50, 30 and 100000, respectively. The maximum depth of each tree refers to the number of rules each tree is allowed to create to come to a decision.

Evaluating regression performance is crucial to understand how well the model is fitted and explained by independent variables. Coefficient of determination (R-squared) and regression error (Re) were the metrics used to detect bias and the proportion of variance of the response variable. A table containing information describing the importance of each predictor used in the model was provided as output by the tool, as well as scatterplots of training data, test data, and test location data, and the regression definition file contains attribute information, statistics, and model performance.

3.2.4. Sensitivity Analysis

Sensitivity analysis was carried out following the process shown in Figure 3.1.

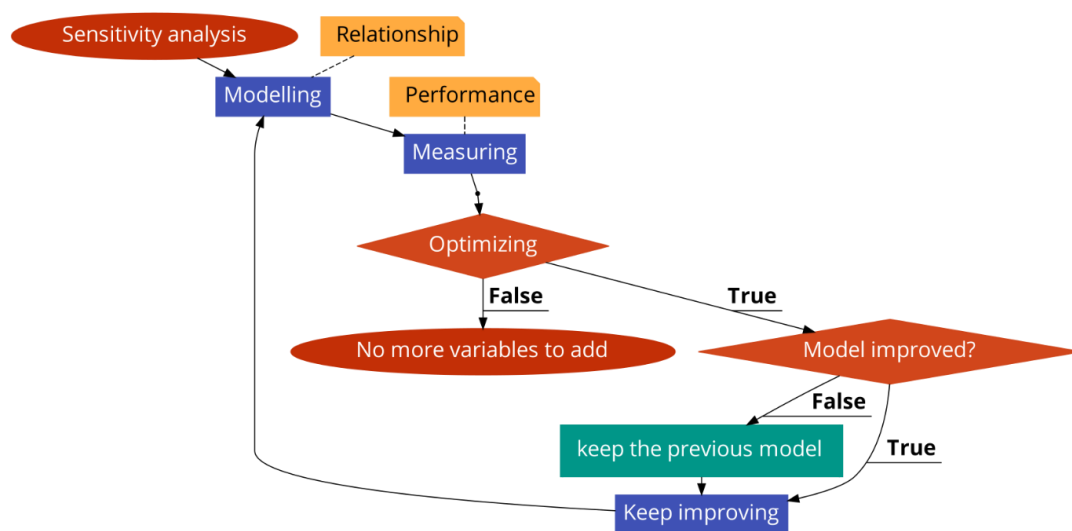


Figure 3.1 - Diagram flow of sensitivity analysis.

The diagram flow has three main steps: modelling the relationship between the response variable and predictors, measuring the model's performance, and optimizing the model. To build the best framework a set of global environmental variables were modelled, the goodness of fit was checked, and the model was optimized as needed. This process was applied twice, on a satellite image sensed on 25/04/2018 and another on 18/08/2018.

Table 3.2 lists the variables included in each test.

Table 3.2 - Description of the explanatory variables included in each model test.

Model	Exploratory variables
M1	Satellite data (Single bands)
M2	Satellite-derived data (NDVI, NDWI, NDMI)
M3	M1 + M2
M4	M3 + Digital Elevation Model (m)
M5	M4 + Average annual precipitation (mm)
M6	M5 + Average annual potential evapotranspiration (mm)
M7	M6 + Annual aridity index

3.2.5. Models' deployment

The most skilled model resulting from the sensitivity analysis was deployed in two different scenarios. One was applying the framework to model landscape water resources on a Sentinel-2 image sensed on 29/01/2022, called temporal deployment. The second deployment was on an image taken on 23/08/2018 in another area (decimal geographic bounding box - Longitude: west = 350.99 and east = 352.28; and Latitude: south = 38.75 and north = 39.75), what was called a spatial deployment. Satellite-derived indices were calculated for both images to apply the framework.

3.3. RESULTS

3.3.1. Sensitivity analysis

The outputs of the training process were analysed to measure the goodness of predictions. The tool checks for three types of errors: errors on training points, errors on test points, and errors on test location points. Table 3.3 shows the models' performance with values for the regression error (Re) at train locations (80% of all locations) and test locations (20% of all locations), and R-squared for training data, test data and test locations. The models are grouped by image date sensed, where sp refers to the image taken on 25/04/2018 and sm on 18/08/2018.

Table 3.3 - Models performance grouped by image date sensed. Legend: TrTr (training data at training locations), TeTr (test data at training locations), and TeTe (test data at test locations), Re (regression error).

	TrTr		TeTr		TeTe	
Model	Re	R ²	Re	R ²	Re	R ²
M1_sp	1.289	0.960	2.904	0.872	3.913	0.894
M2_sp	1.827	0.924	3.751	0.777	5.258	0.809
M3_sp	1.278	0.960	2.925	0.871	3.908	0.892
M4_sp	1.004	0.957	2.490	0.820	3.413	0.851
M5_sp	0.901	0.961	2.134	0.841	3.001	0.850
M6_sp	0.801	0.962	1.980	0.800	2.706	0.811
M7_sp	0.801	0.966	1.980	0.820	2.827	0.825
M1_sm	1.218	0.954	2.488	0.848	3.541	0.878
M2_sm	1.675	0.909	3.189	0.739	4.491	0.779
M3_sm	1.191	0.951	2.455	0.835	3.431	0.886
M4_sm	0.887	0.953	2.220	0.785	3.108	0.772
M5_sm	0.771	0.958	1.950	0.805	2.652	0.824
M6_sm	0.725	0.962	1.816	0.814	2.571	0.829
M7_sm	0.722	0.962	1.830	0.789	2.490	0.839

The best performance was in model M7 for both dates. Models' predictors were the single bands, spectral indices, topography, precipitation, potential evapotranspiration, and aridity index. The image sensed on 18/08/18 has better results regarding Re than the first image. Figure 3.2 describes the importance of each predictor used in the models. The variables with the highest values are more correlated to the target and more relevant to the model. The values range between 0 and 1, and the sum of the values of all variables equals 1. Topography (DEM) was the predictor that most contribute to both models (M7_sp and M7_sm). The predictors' importance varies widely between models. All variables were shown to be important for the models, except for the single band B2 in the summer model (M7_sm), and B3, B4 and NDMI in the spring model (M7_sp). The top five predictors for the summer were (DEM, NDMI, B11, B8, B12) and for the spring (DEM, B11, B7, Evapotranspiration, B6).

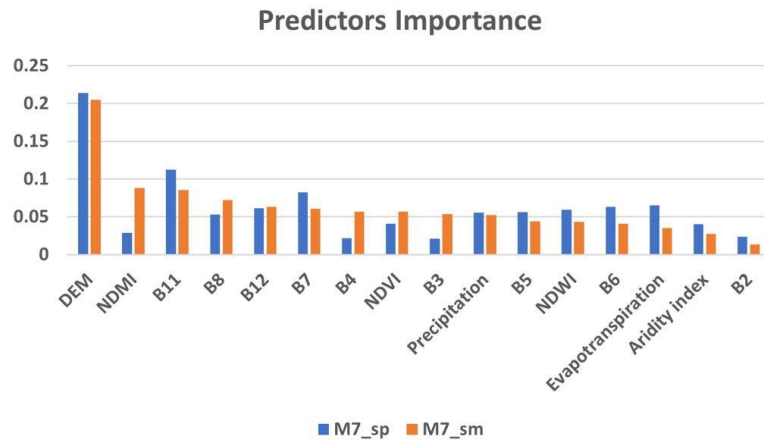


Figure 3.2 - Predictors' importance for the best model in each group of sensitivity analysis tests.

3.3.2. Models' deployment

The framework was deployed to evaluate the temporal and spatial goodness of fit of the selected model. The ML regression tool measured R-squared and regression errors (Re) as the main evaluation measures of the goodness of predictions. The comparison of the true values with predicted values was done in terms of errors (standard error of the regression), the proportion of variance (R-squared) and plotting the residuals over targets. The first deployment was applying the framework at the study area but on another date (29/01/2022). Figure 3.3 displays a scatterplot of predictions over-reference values and the residual plot. The R-squared is comparable with those obtained in the sensitivity analysis, with results showing very closed values, and the residual plot presenting few outliers, especially in the test data at test locations and training locations. What is evident is that in those locations where the WWPI detected no water (WWPI equals zero), this model predicted some degree of wetness. This phenomenon can be explained by analysing the date of imagery, which is from a Mediterranean wet season (29/01/2022), and on that day these locations could be flooded, or the soil moisture was higher than it used to be in the spring and summer.



Figure 3.3 - Scatterplot and residual plot of the temporal deployment applying the framework.

The framework performance was also evaluated by deploying it using a satellite image from another area. Figure 3.4 shows the scatterplot of predictions over observed values and the residual plot of the spatial deployment. Comparing both deployments, the R-squared was better at applying the framework in the same study area rather than applying it to the other region. We also analysed R-squared and Re for test data at training locations and test data at test locations, and the overall results were better in the study area. The residuals present some outliers, but more sparsely than the residual plot of the first deployment.

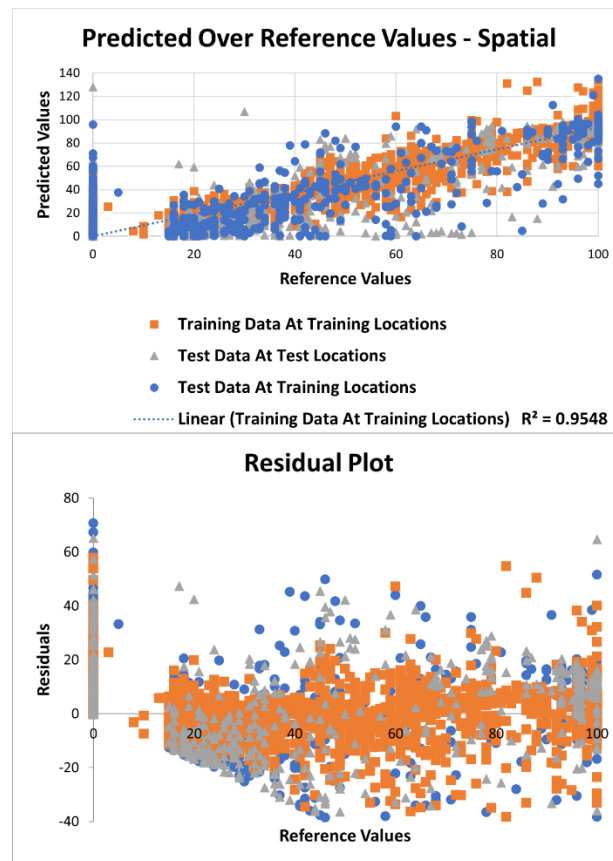


Figure 3.4 - Spatial deployment at the study area applying the framework.

3.4. DISCUSSION

Water diversion and livestock grazing are threatening the functionality of many natural systems, which increases the impacts that a warmer climate may bring. When inland wetlands, rivers, and lakes, get fragmented and become hydrologically inconsistent, the values they produce change, and can rapidly decrease. Assessing water resources at an appropriate management scale is a necessary step for the sustainable management of natural resources.

The HRL developed by CLMS is designed for use by a broad user community as the basis for environmental and regional analyses and for supporting political decision-making (European Environment Agency, 2023). They include geographical information on land cover and its changes, land use, vegetation state, water cycle and earth surface energy variables freely available at the European scale.

They were built based on high-resolution satellite data globally available. High spatial resolution sensors represent a smaller area of land but with more detail and accuracy (Liang & Wang, 2019). However, higher resolution implies larger files, more loading, viewing, and processing time and more space taken up in databases, which can be a limitation. But also building environmental monitoring systems based on ML models requires powerful computational resources, and most of the time a large amount of data.

ML models are only as accurate as the data they are fed in. The most known law of modelling saying, *“garbage in, garbage out”*, could be shown here if we did not carefully select the data to be included in the framework. Large margins of error in the predictors prevent the model from being considered correct. Models with lower error and higher R-squared are indications of higher skill predictions. Nevertheless, none of those functions alone is enough to validate a model’s predictions. Using a combination of evaluation metrics is recommended, to assess the differences between observed data and predictions, to compare models’ performance, and to quantify the explained variance.

Water yield and soil moisture content are some examples of ecosystem functions that are highly dependent on climatic and topographic drivers such as precipitation, evapotranspiration, temperature, and elevation. Topographic variables such as elevation and slope are very important drivers in ecological models. The topography creates specific habitats and influences the occurrence of certain plant species, as in wetlands, an ecosystem that predominantly occurs in flat landscapes, with a very low slope degree. The results show that elevation was the most important feature in both images tested, followed by the single band B11 (SWIR). The shortwave infrared bands highlight water content in vegetation.

The developed framework requires more deployment tests in different locations and time frames. Future work will expand the methodology to assess the relationship between ecosystem services and water resources at the national scale flagging the location and characteristics of water-dependent ecosystems across Portugal. Also, further research is needed to evaluate other ML algorithms and explore other spectral indices and landscape metrics that can be included as reference data in the framework. As well as testing other SEO data such as from the GRACE (Gravity Recovery and Climate Experiment) satellite mission that is used to identify regional trends of freshwater movement on the earth’s surface and compare results.

3.5. CONCLUSION

The framework supports studies related to the spatial estimation of water availability at the European level with the possibility of being implemented multiscale, as it includes global open-access data. The time capability of predictions depends on the launch date of the satellite data used. The comparison of models was important to build confidence in the selected predictors.

The outcomes of this study guide future research to make better use of the globally available data that can be used as predictors in data-driven water modelling. Also, to advance the knowledge of the datasets provided by CLSM at the European level. The developed framework requires more deployment tests, nevertheless, model deployment has shown overall good results and the capability of being used worldwide as a baseline for modelling freshwater ecosystems.

4. A HYBRID MODELLING APPROACH FOR DETECTING SEASONAL VARIATIONS IN INLAND GREEN-BLUE ECOSYSTEMS

4.1. INTRODUCTION

To ensure the long-term viability of Ecosystem Services (ES), it is critical to identify drivers of change and to gather information for their assessment (Meddens et al., 2022). The value of ES is favourably connected with the extent of vegetation and water but negatively correlated with the area of bare land (L. Wang et al., 2021). As competition for land use increases, natural resource management faces new challenges in maintaining GBE functioning and conditions (Doody et al., 2017). Urban sprawl, agriculture practices, and climate change put continuous pressure on natural systems around the world, with ongoing biodiversity losses (Skidmore et al., 2021).

Terrestrial and Aquatic Ecosystems, such as forests, croplands, wetlands, rivers, and lakes provide the most important services in terms of ecosystem provisioning and regulation (Mugiraneza et al., 2019). Commonly referred to as Green-Blue Ecosystems (GBE), the status and functioning of terrestrial and aquatic ecosystems depend on climatic variables, such as precipitation, evapotranspiration, solar radiation, wind, and other variables included in the carbon and water cycles (Gwal et al., 2020). GBE health and behaviour are also influenced by terrain conditions and the presence of groundwater, such as phreatophyte vegetation that requires water on a permanent or episodic basis (Dwire et al., 2018). Seasonality has a substantial impact on these ecosystems during dry periods with little rain, high temperatures and evapotranspiration. As a result, seasonal wetlands dry out while permanent wetlands decrease in extent, vegetation heterogeneity and crop production diminish as well as water yield (Kundu et al., 2022).

The association between aquatic and terrestrial ecosystems are usually observed within rivers that are surrounded by vegetation (Bertrand et al., 2012), and where there is recharge and discharge of groundwater from and to water bodies (Eamus & Ray, 2006). It is strongly influenced by biophysical parameters, such as climate, hydrology, topography, and human activities (X. Yang & Liu, 2020). Groundwater over-abstraction, land-use conversion, climate change, and climate variability are important drivers to explain changes in GBE (L. Wang et al., 2021).

Satellite Earth Observation (SEO), Geographical Information Systems (GIS) and Machine Learning (ML) provide environmental managers and decision-makers with a wide range of tools to assess and monitor ES (Alarcon Blazquez et al., 2023). SEO technology gives a more in-depth perspective for studying land use and land cover change on the earth's surface, as well as a big source of data for evaluating ES values, which is critical for environmental protection and national ecological security (L. Wang et al., 2021). The integration of SEO data with ML is one of the most promising approaches to developing timely and accurate environmental monitoring systems (Reddy, 2021). Traditional ML offers effective techniques for modelling relationships in data with vast feature spaces (Domingos, 2012), but Deep Learning (DL) has been suggested as a better option when it comes to the extraction of significant characteristics from complex datasets (Chang et al., 2019).

The research on the changes in the spatiotemporal aspects of land use and landscape patterns can provide a thorough understanding of the dynamics of the Earth's surface caused by human activities, natural forces, and biological variables over time and space (H. Chen et al., 2021). Therefore, the lack

of guidelines for implementing multi-season satellite-based environmental models is a challenge for those who support decision-making with geospatial information (Doody et al., 2017). More research is needed to determine the association between GBE and biophysical factors utilizing remote sensing data since environmental variables influence the spectral response of ecosystems (Sahana et al., 2022). By reviewing the literature, we identified a common concern about advancing the knowledge of methodologies, tools and strategies that improve the development of seasonal satellite-based data-driven models of GBE, as most research has been focused on specific ecosystem types (green or blue) but not on understanding their relationship.

Recent studies combined SEO and ML to delineate GBE while investigating seasonality effects. Barron et al. (2014) proposed a multi-season method to predict vegetation and waterbodies that can persist through a prolonged dry period, in the Ellen Brook region, an important groundwater basin in Western Australia's south-west. The region is characterized by a Mediterranean climate with GBE associated with localised groundwater, diffuse discharge zones, and riparian vegetation. Mpakairi et al. (2022) investigated the effects of land use conversions and climate change on vegetation heterogeneity in the Khakea-Bray, a transboundary aquifer primarily recharged by precipitation, located between southwestern Botswana and South Africa. The temperature and rainfall in the region are typical of semi-arid savannahs, with high evapotranspiration rates, minimal rainfall during the wet season, and high temperatures during the dry season. Kundu et al. (2022) developed an approach to explore seasonality effects in wetlands in a transboundary river basin (Punarbhaba River) including India and Bangladesh by assessing hydro-period, water depth, and water presence consistency. The study region has a subtropical monsoon climate with seasonal wet and dry spells as well as hot and cold thermal spells. The annual rainfall averages 1500 mm, with 82% falling during the monsoon season (June to September), resulting in the greatest spatial extension of wetlands found during this season. Zhang et al. (2022) classified GBE to assess the status of saline wetlands in the groundwater discharge zones of the Great Plains Aquifer system in eastern Nebraska. In this area, the growing season of wetland vegetation is defined as continuous temperatures above 0 °C from April to October, with the highest water availability in the Autumn and the lowest in the Summer. However, to the best of our knowledge, there is no research investigating the seasonal influence in mapping GBE and estimating their magnitude and relationship in the Lower Tagus Aquifer system. We argue that adopting a hybrid modelling strategy that includes DL and classical ML, as well as hyperparameter optimization, sensitivity analysis, and Feature Importance Estimates (FIE), could close this gap.

The rationale of this study relies on what previous research noted concerning dealing with large datasets and combining techniques to take advantage of each method. When handling large datasets, it is crucial to employ strategies that ensure efficient management and analysis and select optimized algorithms that allow for more efficient processing. Thus, the main aim of this research is to overcome these concerns by developing a hybrid modelling approach to map GBE and estimate their relationship considering seasonality. We propose a two-step modelling strategy that helps to manage and analyze effectively large geospatial datasets while enhancing overall efficiency in GBE mapping workflows.

In the context of climate change, Portugal is recognized as a hotspot among the most vulnerable European countries (Novo et al., 2018). Recent studies have shown evidence of climatic changes, such as the long periods of drought recorded in 1990, 2004/2005 and 2012 (Coelho et al., 2013; de Lima et al., 2015; Almeida and Cabral, 2021). The more frequent occurrence of these events is increasing the severity of seasonality effects on GBE and compromising the provision of services such as freshwater

supply, and consequently crop production, and carbon storage and sequestration (Rijal et al., 2021). The selected study area is within a vulnerable groundwater body (Novo et al., 2018), the Lower Tagus Aquifer system located in the surroundings of Lisbon, the most populated and dynamic area of mainland Portugal (Eurostat, 2023).

Findings from this research can contribute to improving understanding of how these natural systems can be modelled while considering land use dynamics, groundwater depth, and topography to investigate the impact of seasonality on mapping GBE. The purpose of this study is to unveil the potential of SEO and ML in monitoring the response of GBE to seasonal changes and assessing land cover dynamics.

4.2. MATERIALS AND METHODS

4.2.1. Study area

Climate change, drought intensification, deforestation, erosion, desertification, urbanization, rural abandonment, and uncontrolled tourist development are jeopardizing Mediterranean ecosystems (Chrysafis et al., 2020). The Mediterranean climate is known for its particular regional characteristics: large seasonal contrast in temperature and rainfall (hot dry summers and mild winters), strong wind systems, intense precipitation, and Mediterranean cyclones (Li et al., 2012).

Like other Mediterranean regions, Portugal is susceptible to extreme climatic events, such as droughts and desertification effects and is one of the European countries that are most reliant on water resources that originate outside their territory (Almeida & Cabral, 2021). The Lower Tagus Aquifer (study area) is in the downstream area of the international river basin districts PTRH5A in Portugal and its correspondence ES030 in Spain (Figure 4.1). These catchments constitute an important source of water for both Mediterranean countries.

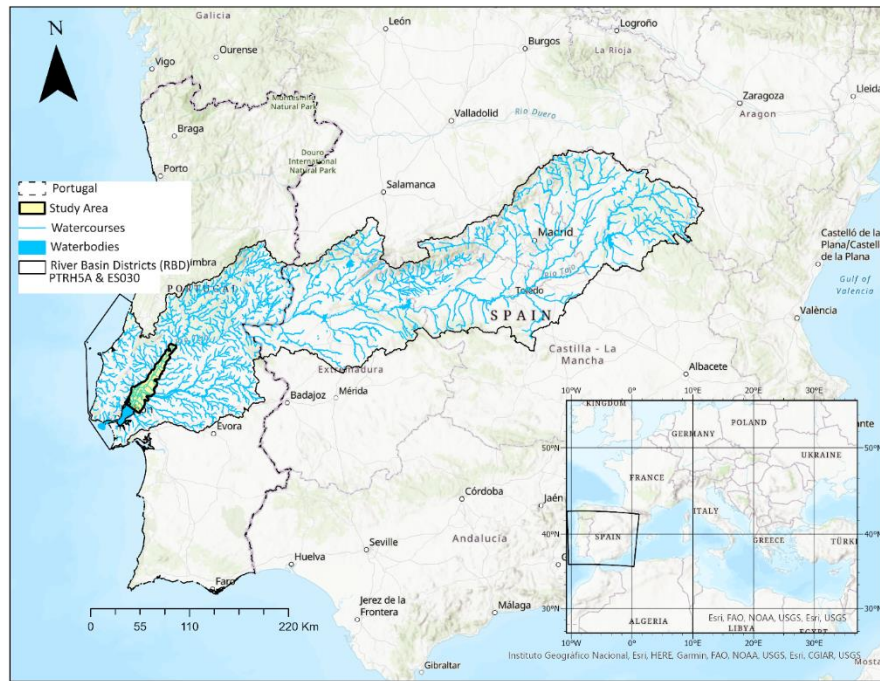


Figure 4.1 - Study area within the transboundary river basins – PTRH5A (Portugal) and ES030 (Spain).

With a length of roughly 1000 km and a catchment area of 80,630 km², the Tagus River begins at a height of about 1600 m in eastern Spain and flows into the Atlantic Ocean near Lisbon (Vis & Kasse, 2009). The river is known for its large size, productivity, quality of its waters, and being responsible for the region's economic and demographic development. The river's proximity to agricultural land facilitates water supply for agricultural intensification (Almeida & Cabral, 2023).

Temporary and permanent crops such as rice fields, and other inundated croplands, vineyards, fruit trees and olive groves are well-developed in the region. Forest and seminatural areas are mostly represented by mixed forest and transitional woodland/shrub, and water and groundwater interactions support the maintenance of ephemeral and permanent wetlands (Ramos et al., 2017).

Precipitation in the Tagus basin has a seasonal cycle, large inter-annual variability, and periodic episodes of extremely wet or extremely dry years (Vis et al., 2010). Spring (March through May) contributes 24% of annual precipitation, Summer (June through August) 6%, Autumn (September through November) 28%, and Winter (December through February) 42% (Belo-Pereira et al., 2011). This strong seasonality in precipitation results in maximum rainfall extreme occurrences (potentially leading to floods) and relatively frequent extended drought spells (Espírito Santo et al., 2014b). Long drought episodes typically cause agricultural damage and alter water resources and availability for many uses (M. M. Oliveira et al., 2005).

4.2.2. Data

Sentinel-2 satellite imagery data with a spatial resolution of 10 m were downloaded from the Copernicus Open Access Hub (<https://scihub.copernicus.eu/>). The modelling process had as input two multispectral images from the Spring (March 26, 2018) and Summer (August 23, 2018) seasons of the Mediterranean climate zone.

Spring and Summer were selected since they are typically the seasons with the lowest average contributions of precipitation, and as a result, less soil water-holding capacity (Belo-Pereira et al., 2011). This is required to distinguish waterbodies from flooded areas (Barron et al., 2014), as major floods that have occurred in the study area since 1980 were throughout the Autumn-Winter season (November to February) (Espírito Santo et al., 2014b), and detect the seasonal variation in the greenness of vegetated land (particularly in the Summer) (Doody et al., 2017). The dates were selected based on the percentage of cloud cover, which was less than 5%.

Satellite-derived indices such as the Normalized Difference Vegetation Index (NDVI), Normalized Difference Moisture Index (NDMI), and Normalized Difference Water Index (NDWI), were calculated. The NDVI was included as a predictor to highlight and distinguish vegetation of different types and at different stages of its evolutionary seasonal cycle (Rouse et al., 1973). The NDMI was employed as it is an indicator of forest change and water stress that enables capturing the moisture differences between land use types (Silleos et al., 2008). Finally, NDWI was used to distinguish water and soil (Gao, 1996) capturing water only in the areas of the deepest channels and with the cleanest water (Ji et al., 2015). The Sentinel-2 derived indices were computed using the following arithmetic functions of bands: (1), (2), and (3):

$$NDVI = \frac{Band\ 8 - Band\ 4}{Band\ 8 + Band\ 4} \quad (1)$$

$$NDMI = \frac{Band\ 8 - Band\ 11}{Band\ 8 + Band\ 11} \quad (2)$$

$$NDWI = \frac{Band\ 3 - Band\ 8}{Band\ 3 + Band\ 8} \quad (3)$$

The reference data for the first-stage modelling is based on the Corine Land Cover (CLC) map of 2018 (spatial resolution of 100 m) (Copernicus Programme, 2023), considering subclasses (CLC Level 3) of agriculture, forest and seminatural areas, wetlands, and water bodies of the CLC Level 1. Surface water and groundwater bodies datasets are from the European Environment Agency – EEA (EEA, 2023) in a version released in the same year. The Digital Elevation Model (DEM), with a spatial resolution of 30 m, is provided by NASA (NASA, 2023) through the Shuttle Radar Topography Mission (SRTM), and the depth of groundwater is derived from the National Information System of Hydric Resources - SNIRH (SNIRH, 2023).

Min-max normalization was applied to the original data to scale the predictors in the range (0, 1) while keeping the relationships between them (4):

$$Xs = \frac{X - X_{min}}{X_{max} - X_{min}} \quad (4)$$

where Xs represents the scaled value of X , X_{min} represents the minimum value of X , and X_{max} represents the highest value of X .

4.2.3. Methods

It is crucial when handling large datasets to employ strategies that ensure efficient management and analysis and implement optimized algorithms that allow for more efficient processing (Nikparvar & Thill, 2021). Besides, instead of loading the entire dataset into memory at once, a good practice is to break it down into manageable parts, or sub-setting the study area.

Automatic classifications with DL can take several hours to complete because training entails the generation of Convolutional Neural Networks (CNN) from the training and validation datasets, requiring the implementation of parallel processing techniques to speed up the analysis. For that, an NVIDIA Graphics Processing Unit (GPU) was configured before training to distribute the workload across multiple cores allowing for faster computation and analysis of the data. The graphic card used in this task is the GEFORCE RTX30 with 16 GB of dedicated memory.

The present approach proposes a hybrid method combining DL and traditional ML algorithms in a two-step process to take advantage of the strengths of each technique. Figure 4.2 shows the flowchart diagram of the modelling process.

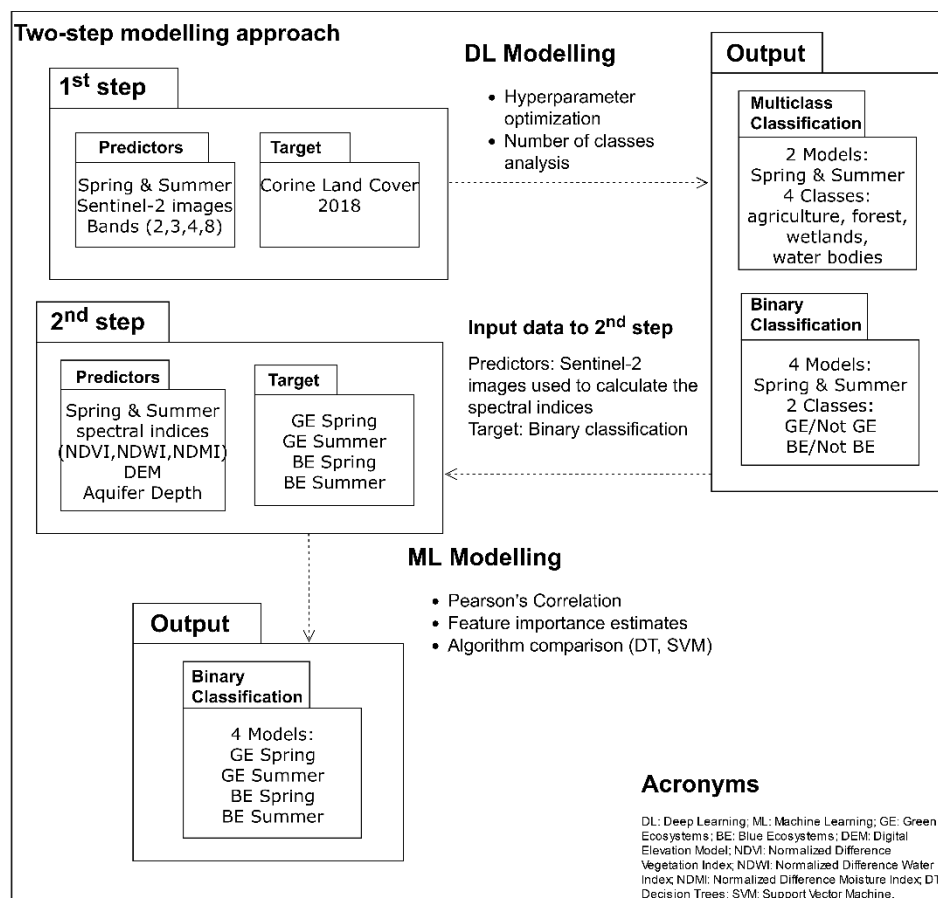


Figure 4.2 - Overview of the methodology development.

The goal of the first step of modelling is to classify land use by seasons with maximum accuracy. Multiclass and binary classifications will be performed using Sentinel-2 bands (2, 3, 4 and 8) and DL. Sensitivity analysis tests and hyperparameter tuning will be used to choose the best models.

In the second step, the main objective is to classify green and blue ecosystems (GE and BE) by seasons, using as input data the binary classification of GE and BE, spectral indices (NDVI, NDWI and NDMI), topography and depth of groundwater (GD). The final models will be presented and discussed with a performance comparison between ML methods. Exploratory analysis and FIE will be carried out to estimate the relationship between predictors of GE and BE by seasons, and then assess which variables contribute the most to classifying GBE. This strategy allows to work with subsets of the data, reducing memory usage, and improving processing speed, and overall efficiency.

4.2.3.1. First-step: DL Modelling

DL via neural networks uses stacked layers to enhance learning by building up representations of the input data in consecutive layers (Guo et al., 2021). To deal with data that needs to preserve its sequence, CNN is the recommended method (Zeiler & Fergus, 2013). This is a technique that convolves the input data to combine successive values to extract higher-level features (LeCun et al., 2015). It has also shown excellent performance in extracting objects from images through down-sampling (Lobert et al., 2021). Utilizing deeper and, therefore, more powerful networks only became possible in recent years through methodological and technical advancements, such as better training algorithms and more powerful computers (A & S, 2023).

In supervised learning, the training data is known and labelled, allowing for direct improvement of the learner's performance. Labels for the training dataset were created based on the CLC 2018 nomenclature guidelines, considering the land use classes of agriculture, forest and seminatural areas, wetlands, and water bodies included in the CLC level one. The artificial surface areas were used as masks.

Sensitivity analysis is carried out to understand the effects and behaviours in the outputs, testing different input values and hyperparameters of the model. The task started creating the training datasets in ArcGIS Pro 2.9.0 (ESRI, 2022) using the tool *Export Training Data for Deep Learning* to convert the data into a format that can be used in the DL packages. The tool converted the labelled vector data (land use classes) into classified image chips using the metadata format of *Classified Tiles*. The multispectral images (a composite of four bands 2, 3, 4 and 8) generated image chips containing the respective class samples from the labelled vector. A few values for image chip size, *Tile Size* and *Stride* (with and without) were tested to find the best model. This tiling strategy is important for large images, to keep the context in the border of the tiles (Zeiler & Fergus, 2013).

The tool *Train Deep Learning Model*, which accepts as input the output folder of the preceding program, was used for training. Model parameters, such as *Max Epochs* and *Batch sizes* were tested with few values to fit the model. The *Model Type* is the U-Net approach used for pixel-based classification. The U-Net architecture works as an encoder network followed by a decoder (Ronneberger et al., 2015), with the learning occurring at different stages of the encoder (Zeiler & Fergus, 2013). The selected *Backbone model* is the pre-trained classification network *ResNet-34*

trained on the Imagenet Dataset (Krizhevsky et al., 2012). The dataset contains more than 1 million images and is 34 layers deep. The use of a pre-training dataset is a method known as Transfer Learning. The *Learning Rate* is set to be extracted from the learning curve during the training process, and the *Validation size* is 20%.

Classification models need to be evaluated regarding quality and accuracy (Stehman & Foody, 2019). The following metrics are calculated to validate the prediction power of all classification tasks: accuracy, recall, precision, and F1-score. The accuracy is the fraction of correct prediction, recall measures how many of the true positive samples were correctly predicted by the model, while precision measures how many negative samples were not labelled as positive. As a weighted harmonic mean factor, the F1-score is associated with precision and recall, and was the guide to selecting the best model, as it is the best option to measure model quality in imbalanced classification problems (R. F. Zhang & Urbanowicz, 2020). The model's output files are the trained model saved in a PyTorch format, a file containing the model's definition (tile size, classes, and model type), and an HTML file with details about the model's performance.

4.2.3.2. Second-step: ML Modelling

The DL model output is utilized as reference data for the second stage of modelling to differentiate between aquatic and terrestrial ecosystems (GBE) by seasons, with spectral indices (NDVI, NDWI, NDMI), elevation (m), and aquifer depth (GD) (m) as predictors.

This process includes data preparation, exploratory analysis, cross-validation (CV) partitioning, FIE, and accuracy evaluation. Decision Trees (DT) and Support Vector Machines (SVM) were implemented using scikit-learn (Pedregosa et al., 2011). DT divides a dataset into increasingly smaller subgroups using the same splitting decision iteratively (J. Zhang et al., 2019). It can handle nonlinear relationships and mixed predictor categories by default, and it is resistant to outliers and collinearity effects (Osborne & Alvares-Sanches, 2019b). The disadvantage of DT is related to accuracy and instability because of error propagation down via consecutive splits in the tree (Breiman, 1984).

The SVM algorithm classifies data by establishing an optimal hyperplane that can divide training data into a predefined number of classes (Boser et al., 1992). The algorithm is based on the principle of structural risk minimization overcoming the problem of overfitting (X. Wang et al., 2021). SVM draw attention due to their robustness, accuracy, and suitability for small training data. However, SVM takes longer to perform, particularly with large datasets (Khwarahm, 2021).

To avoid any data leakage before completing other processes, a 10-fold stratified data partition (CV) is carried out for both ML models. Two filter algorithms, the mutual information (MI) (Peng et al., 2005) and MultiSURF (Urbanowicz et al., 2018) (a Relief-based feature selection algorithm) are used to score the importance of a feature based on how well a feature's value distinguishes samples that are like one another but belong to distinct classes (Pudjihartono et al., 2022). MI is proficient at analysing univariate associations between a feature and the target, while MultiSURF is sensitive to feature interactions without evaluating combinations of features and examining only individuals very near and very far from one another (Urbanowicz et al., 2022b).

The same set of functions used to assess models' accuracy in the first stage is used to evaluate predictions in this step, except the ROC-AUC which is the metric added in this stage. A Receiver Operating Characteristic (ROC) curve is a graph that depicts a classification model's performance across all categorization levels. The AUC (area under the ROC curve) is a function of recall and translates models' accuracy. AUC values close to one mean better-performing classifiers and higher discrimination ability (Mouta et al., 2021).

Statistical comparisons of algorithm performance applied Kruskal-Wallis one-way analysis of variance to determine if any ML algorithm or datasets yielded significantly different performance than the others for each evaluation metric (Urbanowicz et al., 2022b). For any metric where a significant difference is observed, Mann-Whitney U-tests and Wilcoxon Rank test will be calculated to identify which algorithm yielded significantly better or worse performance. The Kruskal-Wallis (Kruskal & Wallis, 1952) is a nonparametric statistical test that compares the differences in a single, non-normally distributed continuous variable between three or more independently sampled groups. The Mann-Whitney U test compares two groups based on a single ordinal variable with no specified distribution (Mann & Whitney, 1947; Wilcoxon, 1945). The null hypothesis states that the n populations sampled have all the same average, whereas the alternative hypothesis states that at least one sample comes from a distribution with a different average.

4.3. RESULTS

4.3.1. First-step Modelling

A land cover classification mapping GBE in the study area is the main outcome of this first-stage modelling. Sensitivity analysis is an integral part of the models' development, involving an analytical examination of the model's settings such as *Max Epochs*, *Batch size*, *Tile size*, *Stride*, and the number of classes.

The first sensitivity tests considered the maximum number of land use classes presented in the study area (17 classes), maximum values for *Tile size* and *Stride*, and minimum values for *Max Epochs* and *Batch size*. The best results were obtained when the image chip size in both dimensions (x, y) (*Tile size*) and the distance that separate tiles (*Stride*) were kept to a minimum, combined with a maximum number of iterations (*Max Epochs*) and *Batch size*. Keeping the *Stride* equal to the *Tile size* guarantees no overlapping in the convolutions. Considering all the existing classes in the study area (a total of 17), the model detected six of them. The other 11 classes did not have a representative number of images and features to be modelled with good accuracy. Table 4.1 shows the land cover classes considered in the first classification task, and those final classes selected by the best sensitivity test.

Table 4.1 - Land cover classes used in the classification task, grouped by sensitivity tests. Legend: CLC – Corine Land Cover.

Sensitivity Test	CLC Level 1	CLC Level 3	Label	Detected (*)
First	2	211	Non-irrigated arable land	
		212	Permanently irrigated land	*
		213	Rice fields	
		221	Vineyards	
		231	Pastures	
		242	Complex cultivation patterns	*
		243	Land principally occupied by agriculture, with significant areas of natural vegetation	
	3	244	Agro-forestry areas	
		311	Broad-leaved forest	*
		312	Coniferous forest	
		313	Mixed forest	
		321	Natural grasslands	
		324	Transitional woodland-shrub	*
		331	Beaches, dunes, sands	
	4	411	Inland marshes	*
	5	511	Watercourses	*
		512	Water bodies	
Best	2	242	Complex cultivation patterns	*
	3	324	Transitional woodland-shrub	*
	4	411	Inland marshes	*
	5	511	Watercourses	*

Figure 4.3 shows the ground truth (first column) and predictions (second column) of the summer and spring models' output. These are the results of the first set of sensitivity analyses classifying 17 land cover classes, generating image chips with a size of 224 x 224 px, number of iterations equal to 40 and 100, and batch sizes of 16 and 32.

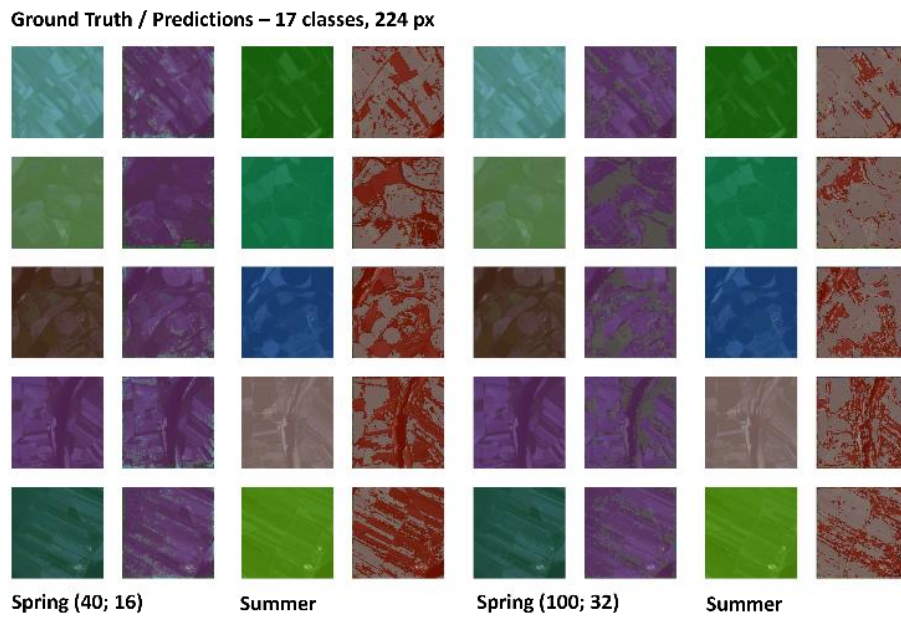


Figure 4.3 - Ground truth and predictions of two different models for both seasons. The models were tested with 17 classes, image size of 224 x 224 px, number of iterations equal to 40 and 100, and batch size of 16 and 32. Legend: Season (number of iterations; batch size).

Decreasing the size of the tiles did not improve the classification accuracy, considering 17 classes. To overcome this, we tested excluding the small classes keeping the most representative samples. After testing with 12, 8, 6, and 4 classes, the best results were considering the following: 242 - complex cultivation patterns, 324 - transitional woodland shrubs, 411 - inland marshes, and 511 - watercourses. Land cover class 242 includes cultivated land parcels with different cultivation types (temporary and permanent crops and pastures) referred to as agricultural areas; 324 represents areas of the natural development of forest formations, transitional bushy and herbaceous vegetation, referred to as woodlands; 411 refer to the wetlands including herbaceous and high floating vegetation in areas usually flooded in winter, or saturated by fresh water all the year; and 511 represents natural or artificial surface watercourses serving as water drainage channels. Figure 4.4 highlights the influence of tile size (64 and 32 px) by comparing ground truth and predictions for both seasons, considering four land cover classes, and keeping the maximum number of iterations (100) and batch size (64).

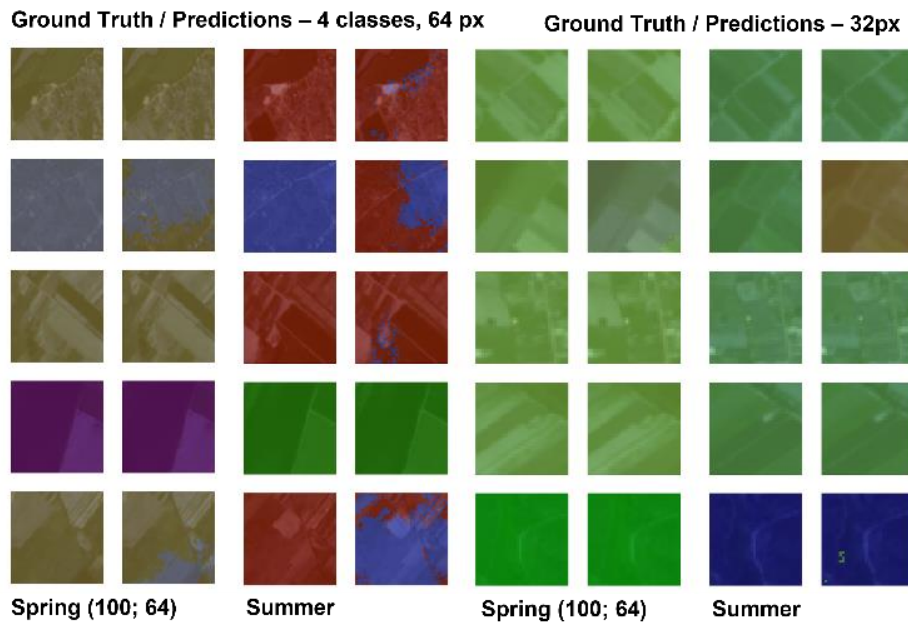


Figure 4.4 - Ground truth and predictions of two different models for both seasons. The models were tested with 4 classes, image sizes of 64 x 64 px and 32 x 32 px, number of iterations equal to 100, and a batch size of 64.

The accuracy of the best multiclass models (four classes, 32 x 32 px image size, 100 epochs and 64 batches, both seasons) is presented in Table 4.2. The models' accuracy was greatest for the spring model, with agricultural areas and watercourses showing the highest results in all metrics, followed by forests and wetlands. The model for the Summer season did not detect wetlands, but classified forests with greater precision than in Spring. The LR slice notation (low; high) represents the combination of low and high values referring to the LR for the first layer and the remaining trainable part of the model, respectively. The LR changes with every iteration. The low and high LR were the same for both seasons, explained by both models' settings configured to complete the iterations, even when the system stopped learning.

Table 4.2 - DL models' performance evaluation summary, considering seasons, the maximum number of iterations and batch sizes (Max Epochs; Batch size). Legend: Land cover classes: 242 – agricultural areas, 324 – woodlands, 411 – wetlands, and 511 – watercourses, LR – Learning Rate.

Type	Model (100; 64)	Class	Accuracy	F1-score	Recall	Precision	LR (low; high)
Multiclass	Spring	242	0.814	0.872	0.932	0.819	1.0965e-05; 1.0965e-04
		324		0.627	0.518	0.795	
		411		0.481	0.354	0.752	
		511		0.785	0.770	0.801	
	Summer	242	0.790	0.862	0.950	0.789	1.0965e-05; 1.0965e-04
		324		0.540	0.402	0.818	
		411		0	0	0	
		511		0.740	0.717	0.766	

The final procedure of this stage was building a binary model mapping GBE. A binary classification task is performed to classify complex cultivation patterns, transitional woodland shrubs, inland marshes, and watercourses into GE and BE by seasons to be used as reference data for the second-stage modelling. The models included a set of 7086 images (32 x 32 px) with 139156 features, *Tile size* (32 px) and *Stride* (32 px). The best models were selected after testing the number of iterations and batch size. Table 4.3 shows the best results for the binary classifications. The Spring model (100;64) showed a better performance than the Summer model for all metrics and tests. The accuracy for the best Spring model (100;64) is 0.876 and 0.866 for the Summer model (100;64).

Table 4.3 - DL models' performance evaluation summary, considering seasons, number of iterations and batch size (Max Epochs; Batch size). Legend: LR - Learning Rate.

Type	Model	Accuracy	F1-score	Recall	Precision	LR (low; high)
Binary	Spring (100; 64)	0.876	0.650	0.576	0.740	9.120e-06; 9.120e-05
	Summer (100;64)	0.866	0.622	0.543	0.729	7.586e-06; 7.586e-05
	Spring (20; 8)	0.876	0.648	0.575	0.743	2.754e-05; 2.754e-04
	Summer (20;8)	0.846	0.529	0.434	0.677	7.586e-06; 7.586e-05

Sensitivity analysis showed that the Spring model did not have a considerable improvement after the 20th iteration, even after increasing the Batch size. While the Summer model needed five times more iterations to show some improvements. Nevertheless, the optimal LR extracted from the learning curve during training was the same for both Summer models. Figure 4.5 shows the evolution through the iterations of the two models' evaluation functions, accuracy, and F1-score. After the 10th epoch, the accuracy for both seasons did not improve much and had very small variations, while the F1-score kept increasing, and did not stabilize before the 80th iteration.

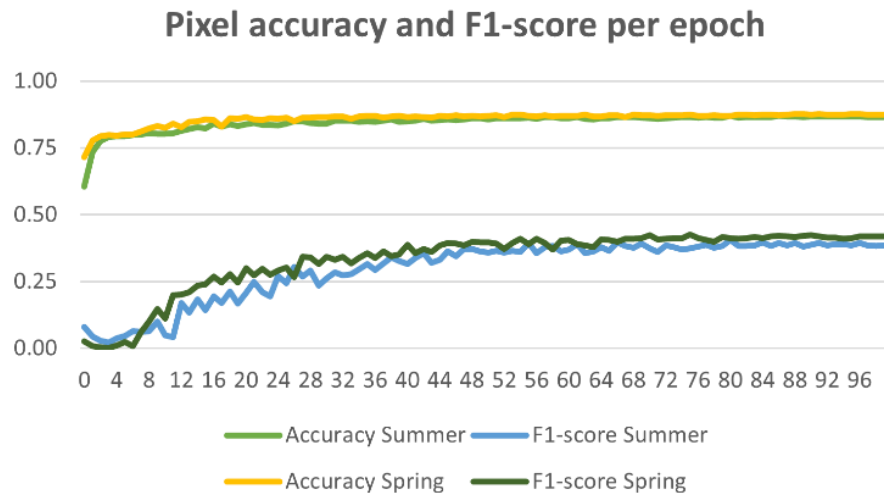


Figure 4.5 - Evolution of models' performance through iterations for both seasons.

The training and validation losses are shown in Figure 4.6. The graph displays the amount of error as the model trained over time. Even though the Spring model has more deviation losses for training and validation (0.050; 0.055) than the Summer (0.037; 0.054), the mean value of losses in the Spring model was (0.390; 0.343) against (0.445; 0.368) for the Summer model. The larger values for the latter are explained by the higher losses verified at the beginning of modelling.

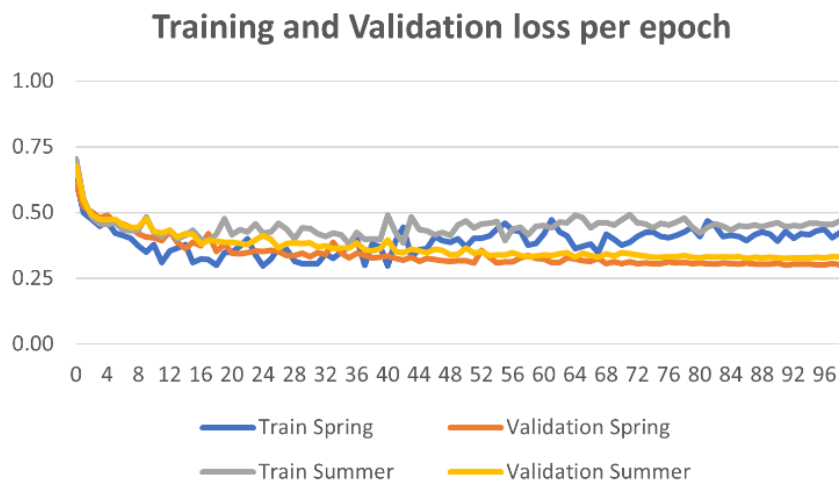


Figure 4.6 - Training and validation loss per epoch for the Spring and Summer models.

4.3.2. Second-step Modelling

4.3.2.1. Exploratory Analysis

The exploratory analysis draws evidence about the relationship between predictors by calculating Pearson's correlation coefficient. The analysed datasets have 14385 instances, five numerical features

(NDMI, NDVI, NDWI, DEM and GD), and no missing values. A scatterplot matrix with correlations and variable distribution for each ecosystem type by season can be found in (A4. Appendix - Chapter 4, Figure A4.1). Table 4.4 summarizes the results of Pearson's correlation by ecosystem type (GE and BE) by season.

Table 4.4 - Pearson's correlation coefficient by ecosystem type (GE and BE) by season. Legend: GE – Green Ecosystems, BE – Blue Ecosystems, DEM – Digital Elevation Model, GD – groundwater depth.

GE Spring	NDMI	NDVI	NDWI	DEM	GD
NDMI		0.803	-0.732	-0.255	0.123
NDVI			-0.969	-0.468	0.196
NDWI				0.467	-0.204
DEM					-0.388
GE Summer	NDMI	NDVI	NDWI	DEM	GD
NDMI		0.795	-0.717	-0.617	0.185
NDVI			-0.964	-0.900	0.293
NDWI				0.966	-0.334
DEM					-0.386
BE Spring	NDMI	NDVI	NDWI	DEM	GD
NDMI		0.791	-0.738	-0.120	0.048
NDVI			-0.963	-0.305	0.132
NDWI				0.326	-0.133
DEM					-0.383
BE Summer	NDMI	NDVI	NDWI	DEM	GD
NDMI		0.753	-0.733	0.118	-0.096
NDVI			-0.950	0.066	-0.049
NDWI				-0.080	0.079
DEM					-0.747

For all ecosystem types and seasons, NDMI showed a high positive correlation with NDVI, and NDWI showed a high negative correlation with NDVI and NDMI. The values for DEM followed a pattern of negative correlation with NDMI, and NDVI, and positive with NDWI, except for BE in the Summer, where the associations oppositely changed. The relationship between DEM and GD was negative for all seasons but for BE in the Summer, the value was twice higher (-0.747). The correlation between GD and the spectral indices also followed a pattern, except for BE in Summer, where the values reversely changed.

The GE Spring model revealed a strong positive association between NDMI and NDVI (0.803), but negative correlations between NDWI and NDMI (-0.732), and NDWI and NDVI (-0.969). The correlation of NDMI and NDWI with topography was at least three times more in the Summer than in the Spring, and NDVI double increased between these seasons.

4.3.2.2. Estimates of Feature Importance

Figure 4.7 compares the FIE between seasons and ML algorithms, for the GE. In the Spring, the DT model estimated NDMI (0.19) as the most representative feature, while SVM predicted NDVI (0.23), but also NDWI (0.18) and NDMI (0.17). In the Summer, SVM and DT estimated NDWI as the most relevant feature and all the other predictors were also considerably weighted, except DEM.

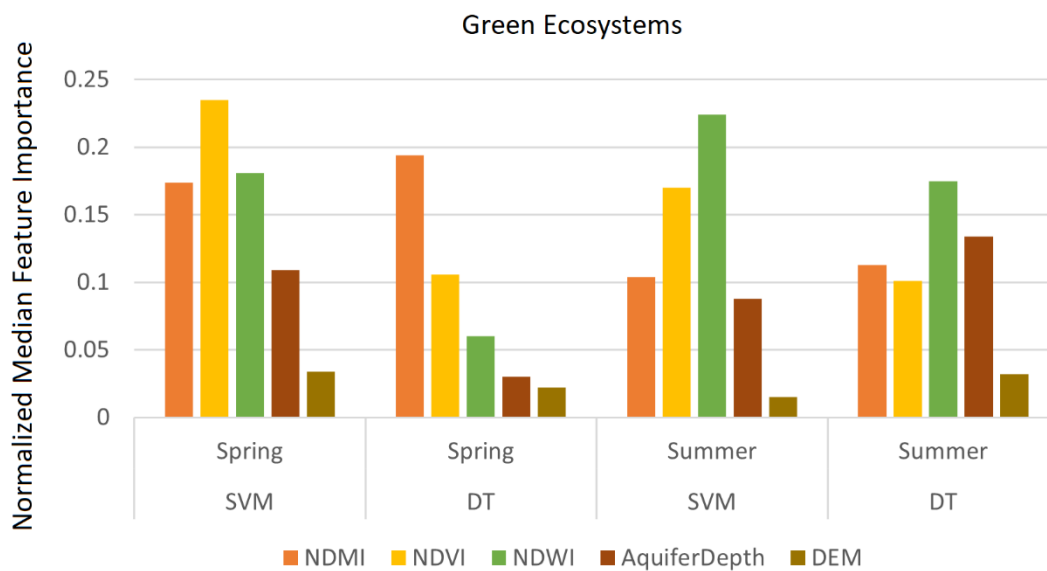


Figure 4.7 - Green Ecosystems feature importance estimates.

For aquatic ecosystems in the Spring season (Figure 4.8), SVM highlighted NDWI (0.18) and NDVI (0.16) as the most relevant variables, while DT homogeneously weighted all predictors, except aquifer depth. In the SVM Summer model, elevation (0.30) and groundwater depth (0.25) were the most important features estimated by those two algorithms. DT excluded NDWI as a predictor in the classification of the BE and did not give much consideration to NDMI and NDVI.

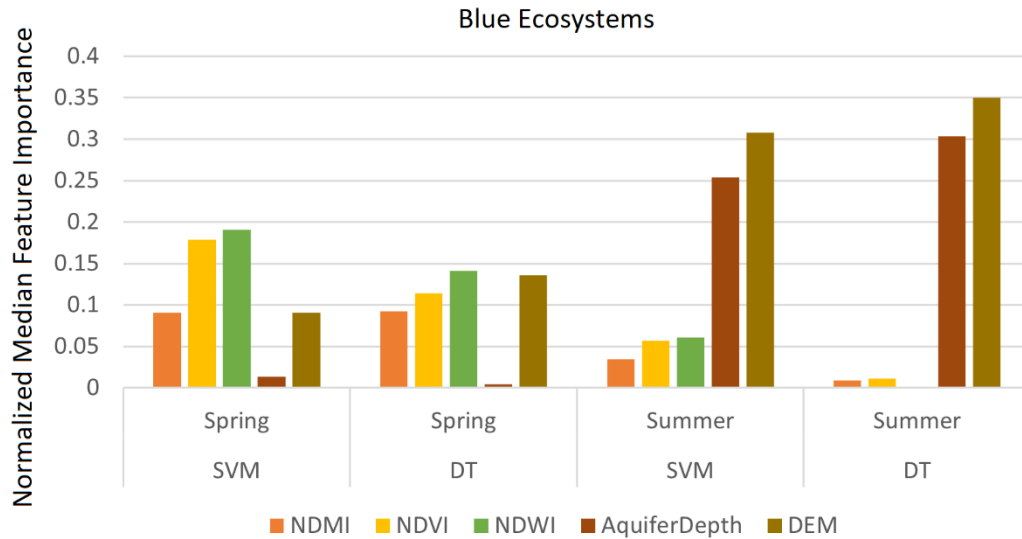


Figure 4.8 - Blue Ecosystems feature importance estimates.

4.3.2.3. Models' performance comparison

Table 4.5 displays the comparative performance between SVM and DT models. The overall results point out that SVM performed best, with all values greater than those obtained using the DT algorithm. The GE Spring model overcomes the Summer results regarding precision. The GE Summer model shows higher values for accuracy, recall, and F1-score. The BE Summer model performed better than the BE Spring in all accuracy functions.

Statistical comparisons of algorithm performance applying Kruskal-Wallis one-way analysis of variance to determine if the algorithms yielded significantly different performance for each evaluation metric. The Kruskal-Wallis significance results compare algorithms for each metric/dataset combination, showing that accuracy, F1-score and recall were significantly different in the GE Spring and Summer models. ROC-AUC is significantly different for GE Spring, and BE Spring and Summer models, and F1-score and precision for BE Spring.

Where these differences were observed, the Mann-Whitney U-tests and Wilcoxon Rank test were calculated to identify which algorithm yielded significantly better or worse performance, but any of these tests was significant to point out a single 'winner' algorithm across all metrics.

Table 4.5 - Models' performance values. Legend: Significance level set at 0.05. Sig(*).

Model	Algorithm	Accuracy	F1-score	Recall	Precision	ROC-AUC
GE Spring	SVM	0.781	0.870	0.781	0.984	0.861
	DT	0.738	0.842	0.739	0.979	0.788
	Statistic	3.857	3.857	3.857	2.333	3.857
	P-Value	0.049	0.049	0.049	0.126	0.049
	Kruskal-Wallis Sig(*)	*	*	*		*
	Whitney U-tests Sig(*)					
	Wilcoxon Rank Sig(*)					
	SVM	0.807	0.886	0.812	0.976	0.832
	DT	0.774	0.864	0.776	0.975	0.826
	Statistic	3.857	3.857	3.857	0.428	0.428
GE Summer	P-Value	0.049	0.049	0.049	0.512	0.512
	Kruskal-Wallis Sig(*)	*	*	*		
	Whitney U-tests Sig(*)					
	Wilcoxon Rank Sig(*)					
	SVM	0.800	0.366	0.785	0.238	0.875
	DT	0.781	0.334	0.747	0.216	0.825
	Statistic	1.190	3.857	0.428	3.857	3.857
	P-Value	0.275	0.049	0.512	0.049	0.049
	Kruskal-Wallis Sig(*)		*		*	*
	Whitney U-tests Sig(*)					
BE Spring	Wilcoxon Rank Sig(*)					
	SVM	0.935	0.689	0.980	0.532	0.982
	DT	0.929	0.665	0.965	0.507	0.975
	Statistic	0.784	1.190	2.333	0.428	3.857
	P-Value	0.375	0.275	0.126	0.512	0.049
	Kruskal-Wallis Sig(*)					*
	Whitney U-tests Sig(*)					
	Wilcoxon Rank Sig(*)					
	SVM	0.935	0.689	0.980	0.532	0.982
	DT	0.929	0.665	0.965	0.507	0.975
BE Summer	Statistic	0.784	1.190	2.333	0.428	3.857
	P-Value	0.375	0.275	0.126	0.512	0.049
	Kruskal-Wallis Sig(*)					*
	Whitney U-tests Sig(*)					
	Wilcoxon Rank Sig(*)					
	SVM	0.935	0.689	0.980	0.532	0.982
	DT	0.929	0.665	0.965	0.507	0.975
	Statistic	0.784	1.190	2.333	0.428	3.857
	P-Value	0.375	0.275	0.126	0.512	0.049
	Kruskal-Wallis Sig(*)					*

4.4. DISCUSSION

Overall, this research was motivated by limitations acknowledged in previously published studies regarding the deployment of multi-season satellite-based models to categorize GBE and establish the

link between drivers. Few studies have investigated the response of GBE to seasonality, such as Barron et al. (2014), Mpakairi et al. (2022), Kundu et al. (2022) and Zhang et al. (2022), but none have gone so far as this research to develop a hybrid approach to classify GBE and understand the relationship between ecosystems, seasonal climate, and groundwater presence. The comparison between seasons captured the effects of seasonal climate variation and relationships between GE and BE. In dry periods, forests, lakes and rivers, and wetlands tend to show water stress, but if they have access to water sources, such as groundwater, the impacts between seasons tend to be less.

Seasonal GBE mapping has been studied in various parts of the world, often limited to local-scale investigations or specific climatic zones. Our study focused on analysing similar approaches carried out in river basins or aquifer systems that commonly experience dry events and understanding and overcoming their main challenges. The findings agreed with previous research as vegetation uses groundwater more during the driest season of the year when alternative water sources become depleted and evapotranspiration demand increases (Aldous & Gannett, 2021).

During the first stage of modelling, a set of sensitivity analysis tests was performed to understand which hyperparameters influence models' accuracy and to identify important uncertainty sources. Sensitivity analysis involves an analytical examination of the input data and hyperparameter settings. The sensitivity tests increased our understanding of models' behaviours and improved models' predictions. The use of this technique helped to provide guidance for future research and produce more accurate models. The outcomes of this step can stand alone as an efficient method to classify land cover (multiclass and binary) using DL in ArcGIS Pro but also can be used in an integrated approach, as proposed in this research.

The results also showed that the DL classification models (Spring and Summer) performed better considering a smaller number of classes, and a higher number of iterations and batch sizes. These models performed slightly better using the Spring dataset to classify transitional woodland shrubs, wetlands, agricultural areas, and watercourses than using the Summer dataset, which did not capture wetlands.

A good example of wetlands in the study region is the protected area Paul do Boquilobo Nature Reserve, a Biosphere Reserve recognized by UNESCO since 1981. It includes inland marshes with areas saturated with water long enough to promote aquatic processes. The DL Spring model was able to delineate seasonal wetlands, discriminating the inland marshes class. The DL Summer model could not differentiate wetlands from the other classes. Instead, it classified seasonal wetlands as a mix of herbaceous vegetation and surface water. Barron et al. (2014) also reported difficulties in the delineation of wetlands in a groundwater basin in the south-west of Western Australia, as these ecosystems are mostly dependent on long-term hydrological regimes. In their study, it is claimed that their approach is better suited for mapping GBE in places with a distinct and extended dry season, with an overall classification accuracy varying from 59% to 91%, which is in line with our results, ranging from 73.80% to 93.50%.

The second-stage modelling provides advanced understanding through exploratory data analysis, assessing the spatial-temporal distribution of GBE and estimating the relationship between ecosystem types, predictors, and seasons. FIE demonstrates the novelty of combining satellite-derived indices, topography, and aquifer depth to improve the model's quality. The comparison between ML algorithms expanded our knowledge and pointed out baselines for future research.

Spectral indices (NDVI, NDWI, and NDMI) showed high positive and negative associations, in all models. Topography presented relevant associations with the spectral indices particularly when modelling GE in the Summer season. In the BE Summer model, aquifer depth and elevation were highly negatively correlated with each other. This contrasting relationship was expected in the study area in this season, as the surface water yield depends on the groundwater level (Almeida & Cabral, 2023). This relationship between drivers aids in the delineation of areas with a higher moisture signature at the surface and the detection of thermal anomalies, which are often linked to a higher level of water availability in groundwater discharge zones. Large changes in climatic conditions, along with continued groundwater abstraction, may result in large variations in groundwater discharges to rivers, springs, and wetlands, causing impacts on the extent of GBE.

FIE evidenced that satellite-derived indices are efficient in delineating GE in both seasons and BE in the Spring, and topography and the aquifer depth for the BE Summer model. The results are compatible with those presented by Barron et al. (2014) in the Mediterranean climate zone of Australia when interpreting the land surface response to dry from combined changes in spectral indices (NDVI and NDWI). Their findings revealed that GBE are characterized by high NDVI and NDWI values at the start of the dry season, but rapidly decrease as vegetation dries up and the moisture content of the soil falls below the soil field capacity.

The high values of NDVI are also an indication of vegetation heterogeneity as demonstrated in the research carried out by Mpakairi et al. (2022). Their findings revealed that vegetation heterogeneity in a transboundary aquifer located between Botswana and South Africa was higher during the wet season and lower during the dry season, and places with a high water table (e.g., a spring or groundwater seepage) are more ecologically varied than areas with a low water table in arid conditions. These findings also justify the relationship between NDVI and GD in our results. Kundu et al. (2022) utilized NDWI to map water depth, hydro-period, and consistency of water presence in a transboundary river (Punarhaba River) that connects India and Bangladesh. The highest positive NDWI values suggest greater water thickness, which confirms our results regarding the importance of NDWI in mapping GBE in the Spring.

The elevation and groundwater depth are some of the important variables in hydro-ecological models (O'Grady et al., 2011), which was also verified in our results. The topography creates specific habitats that influence the occurrence of certain plant species, and the groundwater depth is a proxy for detecting whether ecosystems can freely access water, periodically or not (Eamus et al., 2006). The water presence has the potential to influence the status of GBE, therefore groundwater draw-down and unsustainable groundwater abstraction are compromising ecological integrity at all levels (Eamus & Froend, 2006b). Kundu et al. (2022) found that water depth is a factor of ecosystem resilience, as many species that like to reside at different depths benefit from deeper water depth.

Performance comparison between algorithms indicates that SVM was better than DT in mapping inland GE and BE in both seasons. These methods are the most used to model complex class signatures (Maxwell et al., 2018). SVM may perform better with imbalanced data, due to its stronger generalization capacity, even with small training sample sizes (Tarantino et al., 2021). While DT has the disadvantage of instability due to the propagation of errors down through subsequent splits in the tree (Breiman, 1984). Zhang et al. (2022) tested six ML algorithms including SVM and DT to classify GBE in the groundwater discharge zones of the Great Plains Aquifer system in eastern Nebraska. Their optimal

model (SVM) achieves an overall accuracy of 99.95% for BE classification, against 93.50% obtained in our BE Summer model. For GE classification, their gradient tree boost model achieves an overall accuracy of 94.07% while here the best accuracy for GE is 80.70%, also with SVM.

Our findings require testing other algorithms and methods, in locations with similar environmental characteristics. The statistical tests did not allow us to choose the best algorithm but evidenced that the performance comparisons within the selected metrics were significantly different. Barron et al. (2014), Mpakairi et al. (2022), and Kundu et al. (2022) refer as a limitation that the large-scale technique may not discover seasonal GBE smaller than 30 x 30 m, suggesting efforts for model development using a finer scale, as the present study does, using satellite imagery with 10 m spatial resolution.

Seasonal changes in the greenness of vegetated land can be linked to phenological patterns of vegetation and climate-vegetation interactions. Because of limited rainfall, semi-arid and arid environments are water-scarce, and vegetation relies on surface or subterranean water (Sahana et al., 2022). The GBE are potentially exposed to climate change because of this (Pandey et al., 2023). Apart from climate and lowering of groundwater level, land cover changes also drive changes in GBE (Mpakairi et al., 2022a). Urban sprawl, population growth, and increased agricultural area demand are the predominant drivers of land conversion (Kundu et al., 2022).

Future work can expand the methodology to assess GBE at the national scale and explore other spectral indices, landscape metrics, and contextual data to flag the location and characteristics of GBE. Classifying GBE by seasons in a two-step modelling approach has the benefit of getting the most out of those techniques and adds value to the modelling process by working with subset types of the data. An alternative way to overcome those concerns and handle those large datasets would be using cloud-based storage and computing resources. Even though depending on spatial and spectral resolutions, the process would also require sub-setting.

Moreover, more research is needed to discriminate seasonal wetlands from flooded areas and shrublands, which may require different approaches as they have different responses in terms of reflectance, water requirements, phenology, and spatial and temporal patterns. Concerns came out under this scenario and must be explored in future studies, such as 1) Would it be necessary to include other bands that are specifically able to capture those unique ecosystems in the Summer, or to use other spectral indices or landscape metrics to highlight them?; 2) Which algorithms would better to capture these seasonal variations in wetlands?; and, 3) Which should be a reasonable scale of modelling to detect them?

4.5. CONCLUSION

The overall aim of the study is to have a better understanding of how GBE systems should be modelled considering the dynamics of land use and seasonal climate effects. The approach uses SEO products to detect seasonal climate variations and relationships in the implementation of seasonal satellite-based data-driven models. The sensitivity analysis advanced the knowledge in applying DL models in complex landscapes using GIS tools. The sensitivity tests showed that the hyperparameter settings are key to building accurate models and maximizing the benefits of each technique. FIE demonstrated the novelty

of applying satellite products with contextual data to empower the model's quality. The findings of this study indicate the feasibility of using an observation strategy to continuously monitor the GBE of the Lower Tagus Aquifer system, as well as in other parts of the world.

STAGE 3: RESEARCH DEVELOPMENT AND IMPLEMENTATION

Climatic variables, such as precipitation and evapotranspiration combined with topography are important drivers in water modelling (Ringersma et al., 2003). Topographic variables are the most common auxiliary non-derived spectral predictors. The elevation and slope are very important variables in ecological models. The topography creates specific habitats and influences the occurrence of certain plant species, as in wetlands, an ecosystem that predominantly occurs in flat landscapes, with a very low slope degree (Almeida & Cabral, 2023). The proof-of-concept stage provides a basis for further replicability of methods at multiple scales. It explored and tested global geospatial data together with SEO data and technologies examining the viability of spatial and temporal data through sensitivity analyses, evaluating the confidence of data and methods building evidence for applicability and certainties level. Furthermore, it proposed a hybrid modelling approach to investigate seasonality effects on mapping GBE, arguing limitations, performance, and the model's calibration. These outcomes guided the development and implementation of methodology at multiscale (country, NUTS III, and municipality levels), divided into two studies (chapters 5 and 6). Chapter 5 presents a comprehensive investigation into the estimation of two indicators of forest, water, and wetlands ecosystem condition, the Tree Cover Density (TCD) and the Water & Wetness Probability Index (WWPI). The methodology includes Reverse Engineering (RE) to redesign and reproduce TCD and WWPI datasets provided by the Copernicus Land Monitoring Services, with the introduction of new data and methods to overcome limitations regarding climate conditions, and applied Ecosystem Accounting to quantify the capacity provision of inland GBE in Mainland Portugal. The techniques utilized include cloud-based supervised classification, regression, and factor analysis through geographical detectors. Results show high accuracy when reproducing both Copernicus products, including global climatic and topographic datasets, as predictors. Chapter 6 presents research investigating the spatial effects of carbon storage and sequestration (CSS) within forest ecosystems by utilizing SEO data and technologies, carbon modelling and geospatial analysis. The intricate relationship between forest diversity and carbon distribution was studied, shedding light on the spatial patterns and variability of carbon storage at the country, NUTS III and municipality levels, between 2018 and 2022. Through multiscale spatiotemporal analysis, this study unveils the spatial heterogeneity of CSS across seven forest types.

Chapter 5: Almeida, B., Monteiro, L., Scimama, P., & Cabral, P. (2024). Climate-driven stock accounts of inland Green-Blue Ecosystems: Coupling the carbon and water cycles via Reverse Engineering and Geodetectors

Chapter 6: Almeida, B., Monteiro, L., & Cabral, P. (2024). Revealing dynamics of carbon storage and sequestration in forest ecosystems: A downscaling approach to support monitoring progress towards sustainable management.

5. CLIMATE-DRIVEN STOCK ACCOUNTS OF INLAND GREEN-BLUE ECOSYSTEMS: COUPLING THE CARBON AND WATER CYCLES VIA REVERSE ENGINEERING AND GEODETECTORS

5.1. INTRODUCTION

Understanding the terrestrial biosphere's functioning requires an assessment of the magnitude and distribution of Green-Blue Ecosystems (GBE) (Crowther et al., 2015). Green Ecosystems (GE) support a considerable amount of global biodiversity, playing an important role in biogeochemical cycles, and providing several Ecosystem Services (ES) such as water quantity and quality regulation, food production, raw materials provisioning, genetic resources, and carbon storage and sequestration (Mulatu et al., 2017). Forest density influences soil and water retention rates, flood regulation, as well as competitive dynamics and habitat suitability for a variety of plant and animal species (Rijal et al., 2021). Blue Ecosystems (BE) provide the backbone of ecosystems, enabling agriculture, and influencing urban development decisions (Newbold et al., 2015). As forests are intricately connected to rainfall and water availability, changes in vegetation cover, as well as poorly planned and managed forests, have significant impacts on the carbon and water cycles, leading to pressures on the environment (Liquete et al., 2011). Extreme weather events and soil and water contamination are perceived as the top risk, directly impacting natural capital and biodiversity, and consequently decreasing human well-being (Lundqvist & Unver, 2018). Knowledge of the interactions between carbon and water cycles is vital for predicting ecosystem responses to climate change, as well as the influence on natural capital (Seddon et al., 2021). Despite significant advances, the coupling mechanisms of these cycles under socio-economic and climatic pressures remain poorly understood (Keith et al., 2021).

Ecosystem Accounting (EA) encompass a statistical framework for quantifying and valuing the interactions between nature, society, and the economy, providing physical and monetary measurements of ecosystem assets (Bateman & Mace, 2020). In March 2021, the United Nations Statistical Commission adopted the System of Environmental-Economic Accounting Ecosystem-Accounting (SEEA-EA) as a baseline to inform policy development by countries. It represents a huge milestone in the history of accounting as “it moves beyond GDP and takes better account of biodiversity and ecosystems in national economic planning” (Edens et al., 2022a). Thus, it is susceptible to shaping the future of the national statistic apparatus toward the inclusion of natural capital (Edens et al., 2022a; Lange et al., 2022). Among the challenges still to be overcome is the substantial wide variety and amount of data required to produce comprehensive accounts (Bordt, 2018; Hein et al., 2020). Besides, extending locally generated ES models to other locations or scales has constraints due to the necessity for parameterization, calibration, and validation, which is sometimes hampered by a lack of ground truth data (Cord et al., 2017; Gosal et al., 2022).

The opportunities associated with technological innovations include the potential for gathering, processing, analyzing and visualizing different types of data, and integrating socio-economic and environmental information (Fleming et al., 2022). Advancements in geospatial techniques, such as satellite imagery, geospatial mapping, drones, and sensors, are viewed as highly promising to improve decision-making on both individual and cross-sectoral levels facilitating the deployment of EA (Farrell et al., 2021). Besides, the increased computational power and the transition towards open-access data

and open-source technologies are significantly contributing to enhancing natural capital accounting (del Río-Mena et al., 2023).

Satellite Earth Observation (SEO) data and technologies, coupled with Geographic Information Systems (GIS), provide advantages such as synoptic and repeated coverage, historical spatial data analysis, and cost-effectiveness (Ramírez-Reyes, Brauman, Chaplin-Kramer, Galford, Adamo, Anderson, Anderson, Allington, Bagstad, Coe, Cord, et al., 2019). Therefore, where data is unavailable, imputation data techniques through statistics and Machine Learning (ML) are employed to fill in missing or incomplete data (Fleming et al., 2022). Additionally, data fusion is commonly applied, integrating information from diverse sources such as monitoring, statistics, modelling, or interviews (Braun et al., 2018). These approaches enable more frequent, and consistent assessment of ecosystem dynamics, regardless spatial scale of analysis (Hossain & Hashim, 2019).

In developing models for quantifying natural stocks, accurate and timely data on the extent and status of ecosystems are critical and challenging to gather particularly due to the dynamic and intricate interactions between water/groundwater and vegetation (Ellison et al., 2017). Significant efforts have been made to unveil the potential of SEO in ES assessments (Willcock et al., 2018), such as the European Copernicus programme powered by the European Spatial Agency (2023). The platform yields free and open access to SEO imagery and datasets, providing insights into the status of natural resources not only for Europe but also on a global scale (Almeida & Cabral, 2023). Among the various products, it provides the Water & Wetness Probability Index (WWPI) and the Tree Cover Density (TCD) to assist in building policy-relevant ecological accounts. The WWPI is a biophysical indicator for freshwater and wetland ecosystems (Ludwig et al., 2019) utilized as a spatial proxy to support environmental mitigation, wetland protection, erosion control, flood monitoring, and streamflow regulation (Vargas et al., 2019). The dataset provides information on the status of BE reflecting their overall quality and conditions (Copernicus Programme, 2023). The TCD is an indicator describing forest ecosystem conditions through a continuous spectrum of crown cover information, population numbers, densities, and wood stocks (Crowther et al., 2015). It is acknowledged as an effective method for environmental analyses, forest management, supporting decision-making, and tracking changes in tree cover losses and gains (G. Chen et al., 2020). Therefore, these products have some limitations due to: a) the availability and quality of SEO data, b) the availability and quality of in-situ data, and c) the influence of climatic and topographic conditions (European Environment Agency, 2023). Satellite mission launch dates restrict SEO data availability, and the quality of imagery is influenced by the atmospheric effects on the light reflected off the Earth's surface and captured by the sensor. Another challenge is the lack of ground-truth data, which is expensive to acquire (Mairota et al., 2015).

Some studies have demonstrated improvements with the integration of climate and topographic variables when assessing GBE. Crowther et al. (2015) demonstrated the strong associations between climatic variables and forest density in their research. Ludwig et al. (2019) combined multi-temporal optical imagery, topographic data, and spectral indices to build an automated wetland mapping detection, based on the WWPI. Madrigal-González et al. (2023) used climatic and topographic characteristics to investigate the relationship between tree density and water availability. Han et al (2021) estimated carbon stock in forests by considering temperature, precipitation, elevation, and soil type as factors. Alqadhi et al (2022) demonstrated the impact of landscape and topographic characteristics on ES capacity provisioning, considering: elevation, slope, aspect, drainage density, and precipitation. However, none of these studies used Reverse Engineering (RE) to reproduce TCD and

WWPI taking into consideration climatic and topographic factors to estimate inland GBE at the national level. RE refers to the process of extracting knowledge or design information from products and subsequently reproducing or recreating them based on the acquired information (Nieves-Chinchilla et al., 2018). Through RE, it is possible to learn about the products, search for inconsistencies, or overall vulnerabilities, and assess whether there is a more efficient way to improve them (Wood, 2009).

In this study, the WWPI and TCD will be modelled within Portugal's mainland in ArcGIS Pro (ESRI, 2023) using the *Random Trees Regression* algorithm, and spatial associations will be analyzed through geographical detectors utilizing the geodetectors package (version: 1.0-4) in R software (J.-F. Wang et al., 2016). EA baselines (Kienast et al., 2009) will be followed to assess the climate-driven stock accounts of forests, water, and wetlands at the national level. The aim is to develop more integrated and updated versions of TCD and WWPI contributing to the broader scientific community by exploring the potential of SEO data and technologies combined with global climatic and topographic open-access data. Furthermore, this research will shed light on the interplay between aquatic and terrestrial ecosystems and foster innovative solutions for assessing the status and conditions of inland GBE. Advancing our understanding of the development of Copernicus products will deepen our knowledge of the replicability and applicability of such datasets in EA.

5.2. MATERIAL AND METHODS

5.2.1. Study area

Portugal is located on the Iberian Peninsula in southwestern Europe, comprising a continental portion and two autonomous regions - the Azores and Madeira archipelagos. Portugal's mainland spans an approximate area of 90000 square km located between 36°57' - 42°9'N latitude and 6°12' - 9°30'W longitude in a climatic Mediterranean region (Beck et al., 2018) (Figure 5.1).

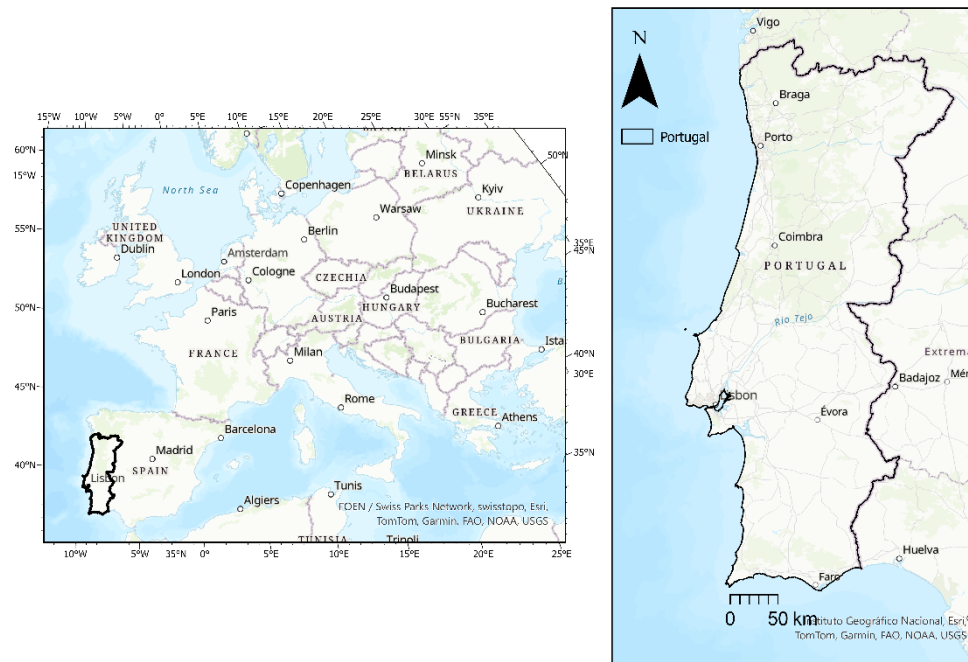


Figure 5.1 - Geographic location of the study area within Portugal's mainland.

The environment changes importantly from north to south, with complex and diverse landscapes (Almeida & Cabral, 2021). Spatial and temporal variability is characterized by latitude, orography, and the effect of the Atlantic Ocean, which affects the water cycle primarily through oscillations in precipitation and temperature (Belo-Pereira et al., 2011). The territory is prone to climate variability, including droughts and desertification, like other southern European regions, notably in the southern sector, which receives the least precipitation and has the greatest temperatures (M. Oliveira et al., 2007).

The climatic conditions, influencing vegetation patterns, contribute to a diverse array of Atlantic, European, and Mediterranean plant species within the country (Santos et al., 2023). Forest ecosystems predominantly consist of broad-leaved and coniferous forests, including Cork oak, Holm oak, Eucalyptus, Maritime pine, and Stone pine (Costa et al., 2022). This ecological diversity is evident across the country, with the northern regions characterized by flourishing broadleaf and coniferous forests like Eucalyptus, Maritime pine, and Stone pine. In contrast, the southern landscape exhibits arid-adapted Mediterranean species such as cork oak, holm oak, and olive trees, representing distinct climatic zones in the country (Fonseca et al., 2019).

5.2.2. Data

Table 5.1 presents the data used in this study, describing their source, spatial resolution, and each dataset's role in the classification and regression tasks. In the GEE platform, cloud-free composites of Sentinel-2 (S2) imagery encompassing the entire mainland of Portugal for 2018 were selected. All available spectral bands from S2 imagery, satellite-derived indices, and topographic features, were employed as classification predictors. These included the Normalized Difference Vegetation Index (NDVI) (Rouse et al., 1973) and the Enhanced Vegetation Index (EVI) (Huete et al., 1997) used to highlight and distinguish vegetation of different types and stages throughout their seasonal cycles; the Soil Adjusted Vegetation Index (SAVI) (Huete, 1988) to mitigate the effects of soil reflectance and

improve vegetation response, and the NDWI (Normalized Difference Water Index) used to differentiate between water and soil, based on the optical characteristics of water (Ji et al., 2015). The S2-derived indices were calculated using the band arithmetic functions: (1), (2), (3), and (4):

$$NDVI = \frac{B8-B4}{B8+B4} \quad (1)$$

$$EVI = 2.5 * \frac{B8-B4}{B8+6*B4-7.5*B2+1} \quad (2)$$

$$SAVI = \frac{B8-B4}{(B8+B4+L)*(1.0*L)} \quad (3)$$

$$NDWI = \frac{B3-B8}{B3+B8} \quad (4)$$

In the formulas, B refers to the spectral band, and L is the soil brightness correction factor that ranges from (0-1). In the SAVI calculation, L takes the value of 0.428, as suggested by Huete (1988). The spectral indices (1), (2) and (3) were used to classify forests, and (4) was employed in the freshwater and wetlands classification.

Topographic variables, such as the Digital Surface Model (DSM) and Slope, were provided by the Japan Aerospace Exploration Agency (JAXA, 2023). These datasets were added with the bands and spectral indices as an 18-band data stack to perform the classification tasks. The classification training datasets included reference vectorial data representing GBE (forest, freshwater, and wetlands) were extracted from the Portuguese land use and land cover map for the year 2018 (COS2018), a national product developed by the Directorate General for Territory (DGT, 2018).

Table 5.1 - Description of datasets utilized in the research. Legend: C - Classification; R - Regression; GEE - Google Earth Engine.

Data	Source	Cell size	Task	Role
Global Digital Surface Model (DSM) (m)	Earth Observation Research Center Japan Aerospace Exploration Agency (JAXA EORC) - GEE	30 m	C	Feature
Digital Elevation Model (DEM) (m) & Slope (SLOPE) (%)	NASA Shuttle Radar Topography Mission (https://www.earthdata.nasa.gov/)	30 m	R	Predictor
Average Annual Precipitation (mm)	WorldClim (https://worldclim.org/)	1 km	R	Predictor
Global Potential Evapotranspiration (Global-PET) (mm)	Consortium of Spatial Information-CSI (http://www.cgiar-csi.org)	1 km	R	Predictor
Global Aridity Index (Global-Aridity)	Consortium of Spatial Information-CSI (http://www.cgiar-csi.org)	1 km	R	Predictor
Satellite imagery 2018 - Single bands	European Space Agency (ESA) – GEE	10 m	C	Feature
Satellite imagery 2018 - Spectral indices	European Space Agency (ESA) – GEE	10 m	C	Feature
Water & Wetness Probability Index (WWPI %) 2018	Copernicus Land Monitoring Services - CLMS (https://land.copernicus.eu/looking-for-national-products)	10 m	R	Response Variable
Tree Cover Density (TCD %) 2018	Copernicus Land Monitoring Services - CLMS (https://land.copernicus.eu/looking-for-national-products)	10 m	R	Response Variable
Land Use and Land Cover Map (COS2018) 2018 (m)	Directorate General for Territory - DGT (https://snig.dgterritorio.gov.pt/)	10 m	C	Target

Climatic variables, such as Precipitation (PREC), Potential Evapotranspiration (PET), Aridity Index (AI), and the Digital Elevation Model (DEM) and Slope (SLOPE) were further utilized as explanatory variables/factors in the regression tasks. Annual PREC was obtained from the WorldClim database (Fick & Hijmans, 2017); Global PET and the Global AI were obtained from the Consortium of Spatial Information, Global-AI and Global-PET Database (Trabucco & Zomer, 2019). Global PET and AI were derived from the WorldClim precipitation model and have the exact spatial resolution and temporal scales.

The response variables (WWPI and TCD) are from the High-Resolution Layers portfolio of the Copernicus. The WWPI is a raster that depicts the presence of water and wet areas as an index ranging from 0 to 100% (Copernicus Programme, 2023). The WWPI workflow includes satellite data fusion, supervised ML classification and an unsupervised thresholding technique for water/wetness detection. Data fusion is based on optical data from S2 and Landsat 5/7/8 and radar data from Sentinel-1 multi-temporal imagery from 2012-2018. The classification task was performed with the RF algorithm, and post-processing included quality assurance, control procedures, visual improvements and error correction. The TCD is a vertical projection of tree crowns onto a horizontal Earth's surface providing pixel-level information on tree cover density (%). In the TCD development, Sentinel-2A+B time series (Level-2A data) were employed to build a supervised classification model using an RF classifier to create a binary Tree Cover Mask (TCM) (all non-tree covered areas/tree cover). Following that, a multiple linear regression was carried out inside the bounds of the TCM to estimate TCD values.

5.2.3. Methods

Forward Engineering goes from concept to product, while RE does the opposite, applying techniques to create a blueprint of an existing product (Vallero, 2014). RE is frequently used to replicate existing products, test, or improve functionalities, and introduce new data (Nieves-Chinchilla et al., 2018). It is defined as the process of examining an object to determine its components and their interrelationships for further redesign and recreation (Wood, 2009). There are a few steps to follow when applying RE, such as defining the purpose, reviewing product specifications, identifying limitations and vulnerabilities, disassembling, analysing, redesigning, and reporting (Chikofsky & Cross II, 2002).

The research development starts applying the RE approach to understand how TCD and WWPI were created, how they work, and how they could be improved, followed by employing the EA framework to quantify the physical measurements of inland GBE, through estimations of ecosystems extent (Figure 5.2a) and condition ((Figure 5.2b). Ecosystem extent quantifies the area per ecosystem type inside an accounting area. In contrast, ecosystem condition records the status of an ecosystem asset through indicators that reflect its condition (United Nations et al., 2021). The extent was estimated through classification tasks mapping GE and BE, while the condition of forest, freshwater and wetlands was predicted by regression tasks. Finally, there was the calculation of factor importance and interaction, and statistic tests between factors and within ecosystems, employing geodetectors.

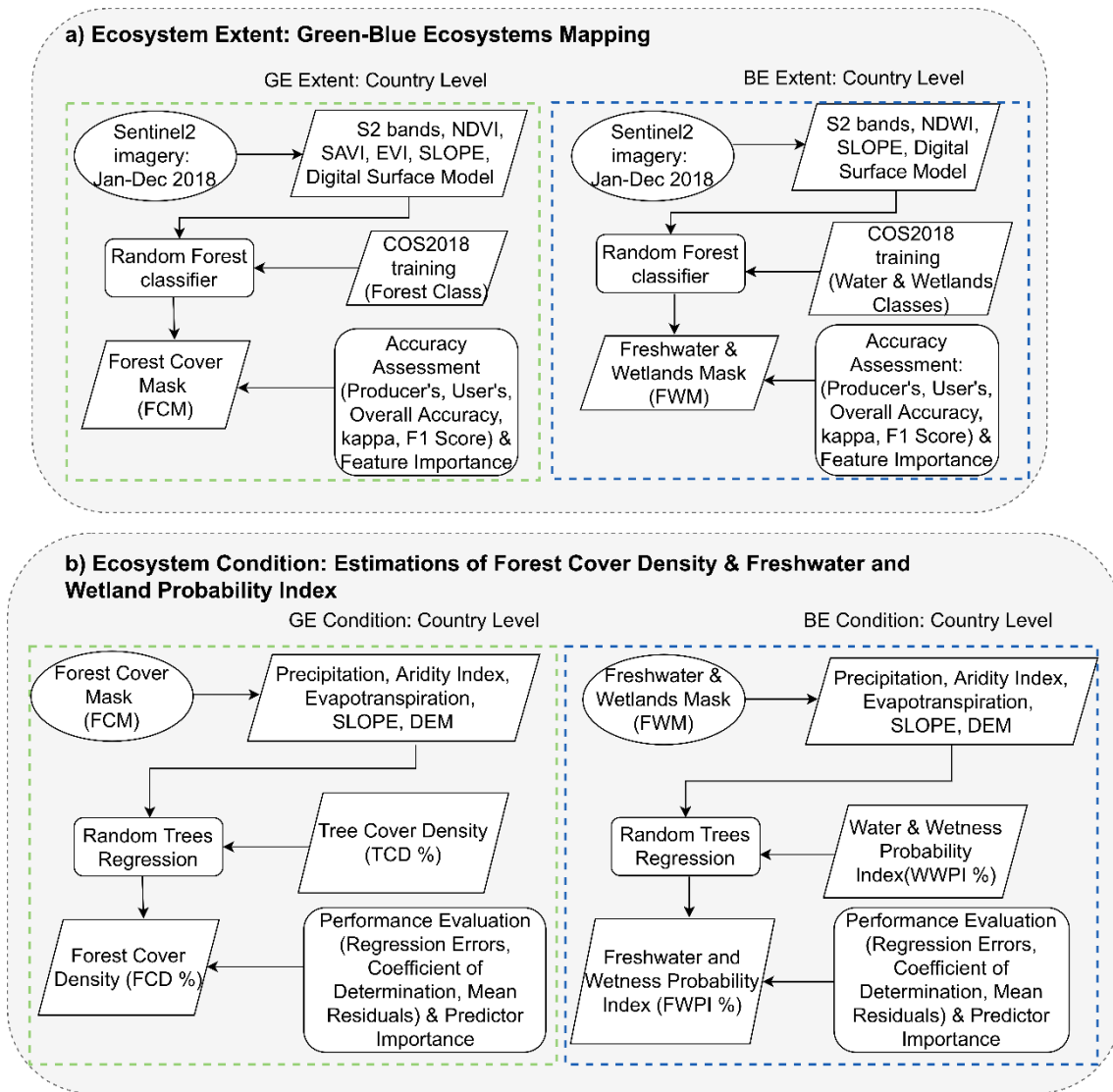


Figure 5.2 - Methodology scheme depicting the estimations of ecosystem extent and condition.

5.2.3.1. Classification task

Two distinct classification tasks were conducted: one dedicated to creating the Forest Cover Mask (FCM) and another to creating the Freshwater and Wetlands Mask (FWM). The training data were extracted from the COS18 dataset and used as samples for a Random Forest (RF) classification (Breiman, 2001), in Google Earth Engine (GEE) (Google, 2023). The scripts are provided in the A5. Appendix - Chapter 5, Tables A5.1 and A5.2.

Random point sampling was employed to provide training and validation data for the tasks. The RF ML algorithm evaluated the training features in terms of S2 single bands and spectral indices, DSM, and slope. Additionally, to optimize the model and improve its accuracy, an analysis of feature importance and hyperparameter tuning was conducted for each classification. These analyses enabled the identification of the most relevant features and refining the RF algorithm, enhancing classification accuracy for each designated class.

The classification result was then subject to an accuracy assessment procedure using the validation points by calculating different metrics, such as overall accuracy (OA), confusion matrix, producers'

accuracy (PA), users' accuracy (UA), kappa coefficient, and F1 score. Lastly, post-processing techniques were applied to eliminate isolated pixels and noise.

5.2.3.2. Regression task

Predictive spatial ML regression was used to model the relationship between explanatory variables and response variables (WWPI and TCD) using ArcGIS Pro 2.9.0 software. The regression tasks were implemented using the tool *Train Random Trees Regression Model*.

The ML spatial regression models for TCD and WWPI were built considering five explanatory variables (PREC, PET, AI, DEM, and SLOPE). The *Percent Samples for Testing* option was set to 20%, which means that one-fifth of the training sample, referred to as test location points, was used to quantify the error for interpolation in space. Three types of errors were measured: errors on training points, errors on test points, and errors on test location points. The *maximum number of trees*, *maximum tree depth*, and *maximum number of samples* were all set to 50, 30, and 100000. The maximum depth of each tree refers to the number of rules that each tree can generate to decide.

It is critical to evaluate regression performance to understand how well the model is fitted and explained by independent variables (Hosmer & Lemeshow, 2000). The metrics utilized to detect bias and the amount of variance of the response variables were the coefficient of determination (R-squared) and regression error (Re). The tool outputs a table describing the importance of each predictor used in the model, as well as scatterplots of training data, test data, and test location data, and a regression definition file containing attribute information, statistics, and model performance.

5.2.3.3. Factor analysis using Geodetectors

Factor analysis was carried out to estimate the drivers of GBE using geographical detectors. Geodetector is a tool for investigating spatial stratified heterogeneity (SSH) through (1) measuring and finding SSH of a variable Y; (2) testing the power of a determinant X of a dependent variable Y based on the consistency of their spatial distributions; and (3) investigating the interaction between two explanatory variables X1 and X2 (J.-F. Wang et al., 2016). The tool is implemented by the geographical detector *q*-statistic (5):

$$q = 1 - \left(\frac{1}{N\sigma^2} \right) \sum_{h=1}^a N_h \sigma_h^2 \quad (5)$$

where N and σ^2 represent the number of units and Y variance, respectively; the population Y is made up of a strata ($h = 1, 2, \dots, a$), and N_h and σ_h^2 represents the number of units and Y variance in stratum h , respectively.

The strata of Y are a partition of Y by a categorical explanatory variable X ($h(X)$) (J. Yang et al., 2022). In this study, the strata refers to each ecosystem, hence the *q*-statistic was calculated for GE and BE. The *q*-statistic value is between [0, 1], then $q = 0$ indicates no relationship between Y and X; $q = 1$ shows that Y is governed by X; and the *q*-statistic value indicates that X explains 100 q % of Y. The *q*-statistic quantifies the relationship between X and Y in linear and nonlinear ways.

The factor analyses were calculated using the R geodetector package (J.-F. Wang et al., 2016). The factor detector *q*-statistic calculates the SSH of a variable Y as the determinant power of a covariate X of Y. The function returns the *q* statistic as well as the respective *p*-value. The ecological detector

determines whether there are statistically significant differences between two risk factors $X_1 \sim X_2$. The F statistic is utilized in this function to test the differences at a significant threshold of 0.05. The interaction detector determines whether the factors interact with Y. The risk detector computes the average values for each stratum of the explanatory variable (X) and shows if there are differences between strata.

5.3. RESULTS

5.3.1. Forest, freshwater and wetlands mapping

A binary classification task mapping forest/non-forest areas was performed at the national scale. Also, a multilabel classification task delineating freshwater and wetlands areas was carried out. Both classification maps are required for the calculation of ecosystem extent and will be employed as masks in the subsequent step, the regression tasks (Figure 5.3).

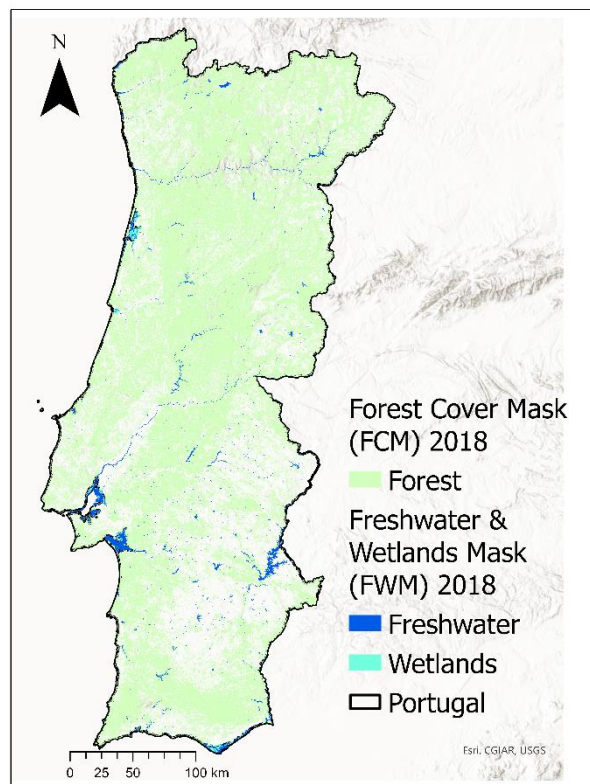


Figure 5.3 - GBE mapping for Mainland Portugal.

The FCM and FWM classifications exhibit high accuracy, strong agreement, and reliability in their respective classifications. Table 5.2 presents the accuracy evaluation for forest classification (FCM) and freshwater and wetlands classification (FWM).

Table 5.2 - Accuracy evaluation. AO: Overall Accuracy; PA: Producer's Accuracy; UA: User's Accuracy.

LULC	OA (%)	PA (%)	UA (%)	Kappa	F1 Score
GE	96.17	93.68	95.71	0.89	0.93
BE	94.66	95.83	96.67	0.94	0.94

The FWM classification achieved an overall accuracy (OA) of 94.66%, while the FCM classification achieved an even higher accuracy of 96.17%, indicating a high level of correctness in their respective classifications. For the producer's accuracy (PA), the FCM classification demonstrated a result of 93.68%, while the FWM classification showed a slightly higher result (95.83%), indicating their ability to identify their respective categories accurately. As for user accuracy (UA), the FCM classification exhibited an accuracy of 95.71%, while the FWM classification demonstrated an accuracy of 96.67%, indicating the reliability of both models' predictions.

The forest cover classification exhibited a robust agreement, boasting a Kappa value of 0.89. The classification of freshwater and wetlands demonstrated an even higher level of agreement, with a Kappa value of 0.94. These results underscore both models' strong consistency and reliability in accurately categorizing vegetation, freshwater, and wetlands. The F1 scores further reinforce the models' effectiveness in correctly identifying these land cover categories. The FCM classification achieved a commendable F1 score of 0.93, while the FWM classification excelled with an impressive F1 score of 0.94. These high F1 scores highlight the models' ability to strike a balance between precision and recall, making them valuable tools for land cover classification tasks. When looking at the mean percentage values of feature importance for the water and wetlands classification at the national level (Figure 5.4), the analysis provided insights into the features crucial for discriminating water bodies and wetland areas accurately. As such, among the 13 attributes assessed, the surface elevation (DSM) exhibited the highest significance (13.65%), followed by NDWI (9.70%) and Slope (9.30%). S2 Bands (8, 11, 12, 8A, 4, 6, 5 and 7) presented importance higher than 5%, while Bands (3 and 2) were less than 5%.

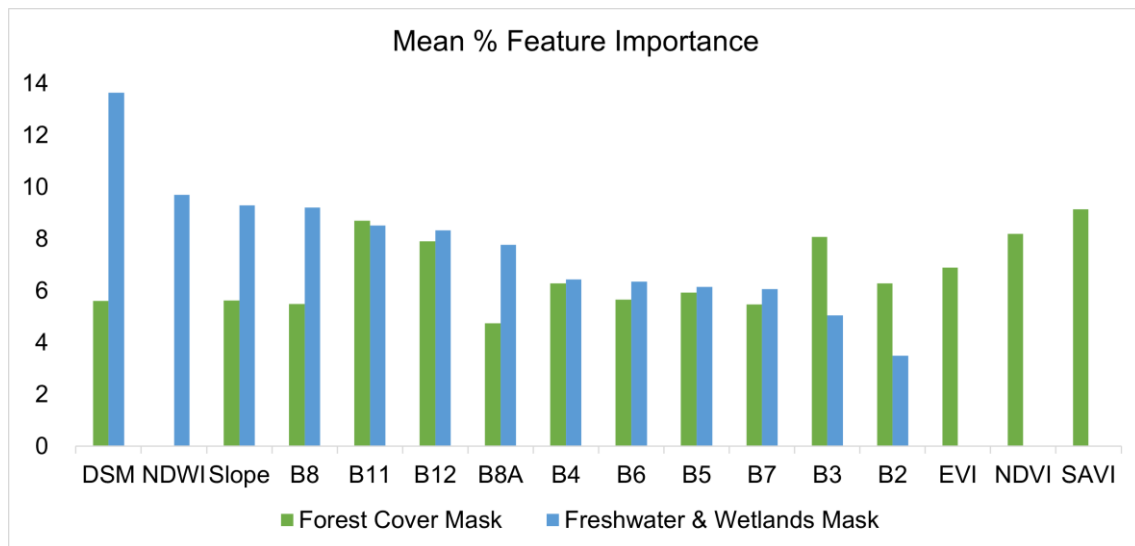


Figure 5.4 - Mean % Feature Importance for Forest Cover Mask (FCM) and Freshwater & Wetlands Mask (FWM).

Regarding the forest cover classification, a total of 15 attributes were considered as predictors. The feature analysis demonstrates that the spectral indices, SAVI (9.14%), NDVI (8.19%) and EVI (6.89%), showcased notable significance, but also S2 Bands 11 (8.70%), 3 (8.09%) and 12 (7.91%). The Short Wave Infrared (SWIR) bands, B11 and B12, capture variations in vegetation water content and the spongy mesophyll structure within vegetation canopies. Meanwhile, B3 is sensitive to healthy vegetation. The S2 Band 8A was the only feature contributing with less than 5%. The S2 Bands (7, 8, 6, 5, 2 and 4), DSM and Slope presented importance values of more than 5% but less than 6.89%.

5.3.2. FCD and FWPI predictions

R-squared and residuals were used to assess the accuracy of FCD and FWPI predictions. The true values were compared to predicted values in terms of proportion of variance (R-squared), and residuals over targets. Figure 5.5 shows the scatterplot of predicted (FCD) over-reference values (TCD), and results for R-squared at training points (Tr), at test points (Te), and test location points (TI), as well as the residual plot. The R-squared at Tr, Te and TI, were respectively, 0.8746, 0.5456, and 0.3208. The R-squared for residuals is 0.4131 and the mean residual value is 0.04. These statistics were calculated using 100000 samples.

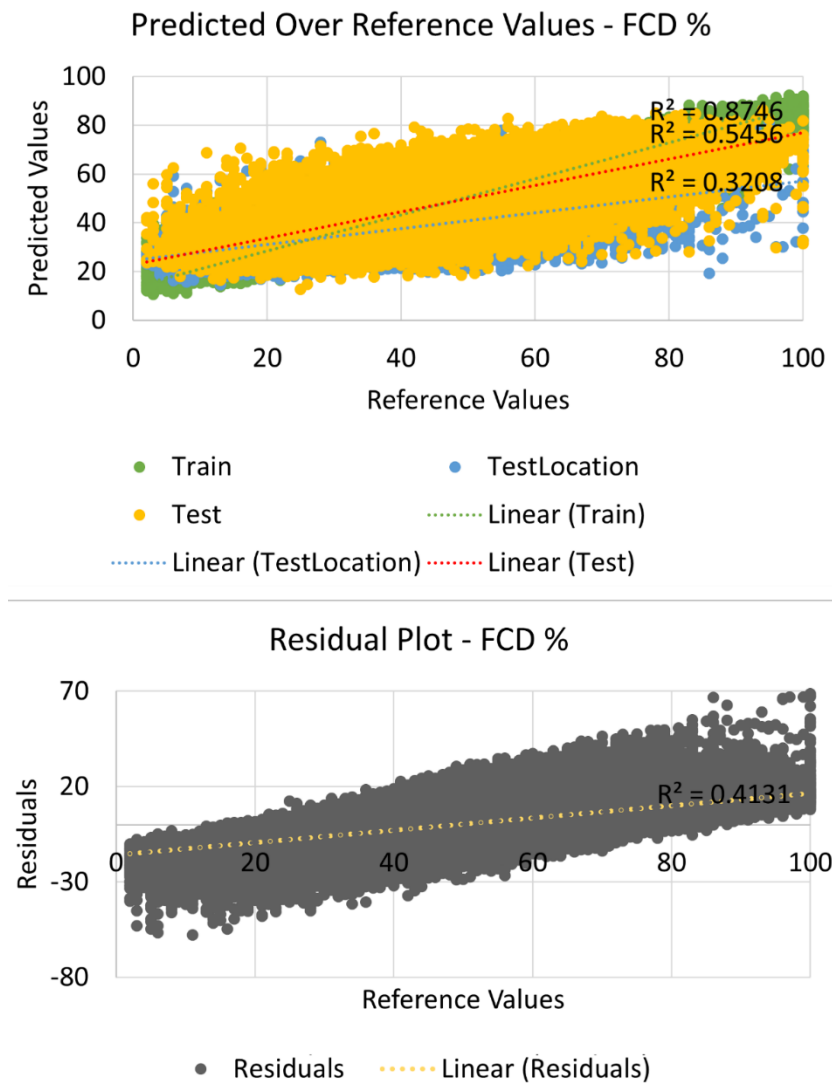


Figure 5.5 - Scatterplot (top) and residual plot (bottom) of the Forest Cover Density (FCD) model.

The scatterplot of predictions (FWPI) over observed values (WWPI) and the residual plot for the FWPI model are shown in Figure 5.6. R-squared values at Tr, Te, and Tl were 0.8275, 0.6153, and 0.6555, respectively. The R-squared residual is 0.4765 and the mean residual value is 0.08. In the predictions of FWPI, the R-squared showcased superior results in Te and Tl. However, FCD performed better than FWPI, as R-squared at Tr is higher, and Tr corresponds to 80% of samples.

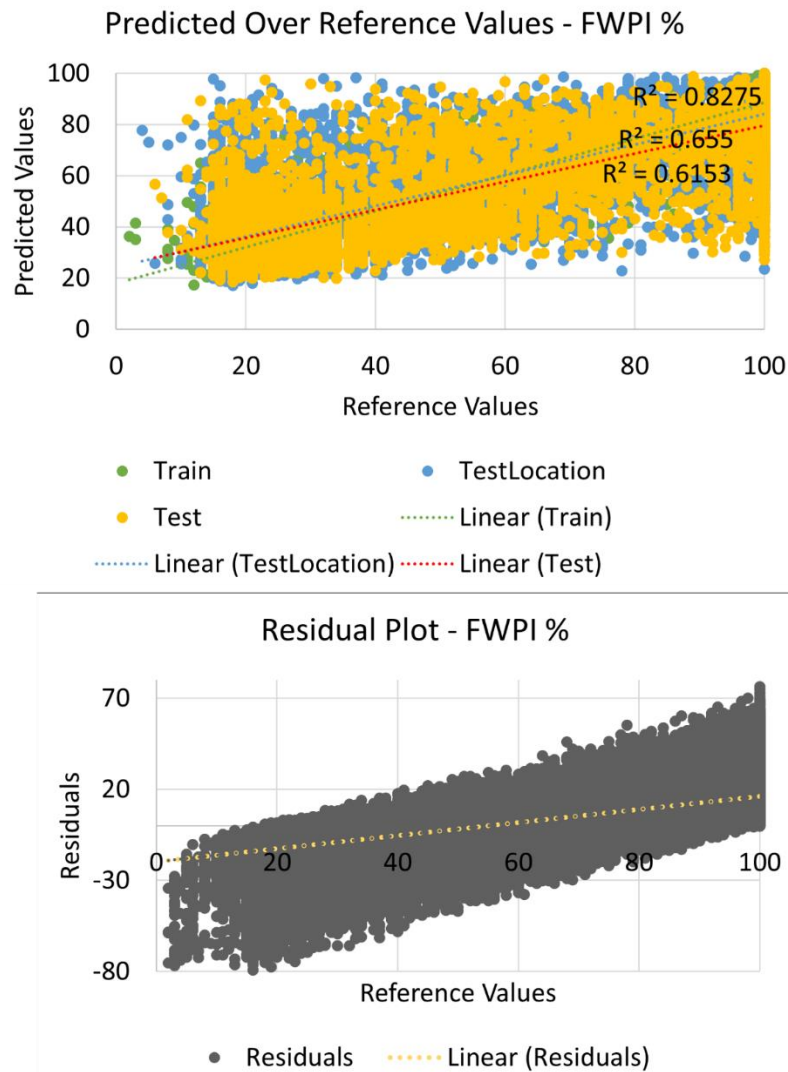


Figure 5.6 - Scatterplot (top) and residual plot (bottom) of the Freshwater & Wetness Probability Index (FWPI) model.

Table 5.3 presents the equations for each sample set (Tr, Te, and Tl) used to assess the model performance.

Table 5.3 - Performance evaluation by model (Tr: Training data at training locations, Te: Test data at training locations, and Tl: Test data at test locations).

Model	Residuals	Tr	Te	Tl
FCD	$y = 0.32x - 15.76$	$y = 0.74x + 13.68$	$y = 0.54x + 22.83$	$y = 0.32x + 24.62$
FWPI	$y = 0.36x - 19.82$	$y = 0.71x + 17.9$	$y = 0.55x + 24.71$	$y = 0.6x + 24.21$

The explanatory variables for both regression models were DEM, SLOPE, PREC, PET, and AI. Figure 5.7 describes the importance of each variable for FCD and FWPI. The predictors with the highest

percentage values were more relevant to the model. All variables were shown to be important for both models, except the SLOPE. DEM and PREC were the factors that most contributed to the FWPI model, followed by PET and AI, and lastly, SLOPE. For the FCD model, PET and AI contributed the most, followed by PREC, DEM, and SLOPE.

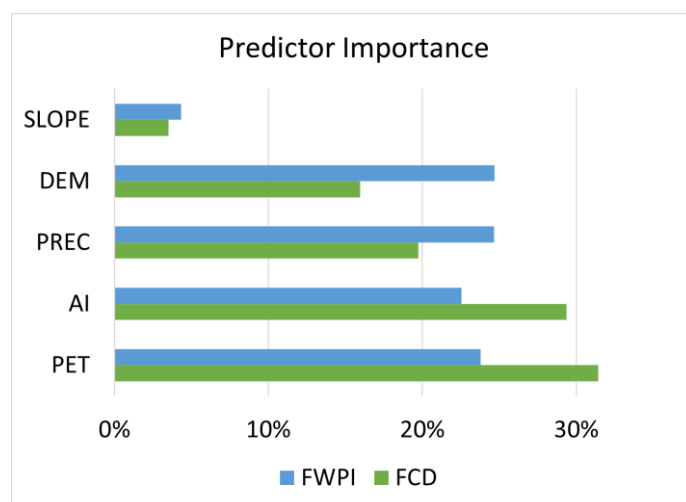


Figure 5.7 - Predictor importance for Freshwater & Wetness Probability Index (FWPI) and Forest Cover Density (FCD) regression models.

5.3.3. Factor analysis using geodetectors

The factor detector q-statistic indicates if explanatory variables stratify Y (GE and BE). Table 5.4 depicts the factor detector results. In the prediction of BE, PREC and AI presented q-values higher than 0.5; DEM and PET higher than 0.25; and SLOPE close to 0, meaning there was no association between FWPI predictions and SLOPE. For GE, PREC and AI show the highest degree of association with values higher than 0.5, followed by PET (0.44), SLOPE (0.13) and DEM (0.11).

Table 5.4 - Factor detector results for Blue Ecosystems (BE) and Green Ecosystems (GE) estimation.

Y	Statistics	SLOPE	DEM	PET	AI	PREC
BE	q-statistic	0.06	0.42	0.29	0.55	0.69
BE	p-value	1	9.04E-10	9.05E-10	9.35E-10	9.19E-10
GE	q-statistic	0.13	0.11	0.44	0.54	0.65
GE	p-value	1	9.50E-10	8.47E-10	9.66E-10	9.36E-10

The ecological detector determines if there are statistically significant differences between two covariates. This function utilizes the F-statistic to test for differences, employing a significance threshold of 0.05. In both GE and BE models, all variables were found to be significantly different.

The interaction detector determines whether the factors interact with the covariate. All interactions between factors had q-values greater than individual factors, demonstrating combining phenomenon-related factors increases the explanatory power of GBE (Figure 5.8). The strongest interactions (greater than 0.75) were observed between AI and PREC (0.83), DEM and PREC (0.82), AI and PET, PET and PREC (0.78), and between DEM and PET (0.75). It was not verified that there were any interactions between AI with SLOPE, AI with DEM, and SLOPE with PREC, but SLOPE interacted with DEM (0.59) and PET (0.53).

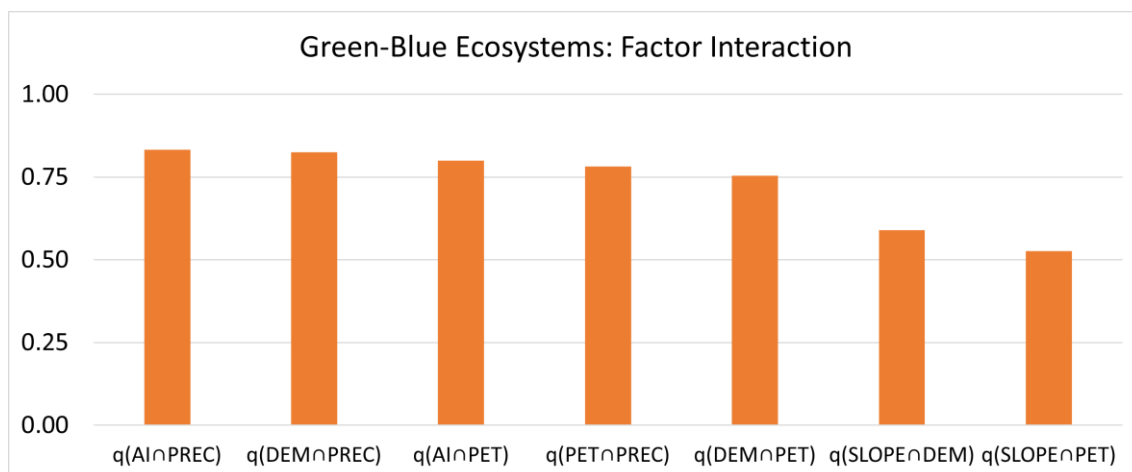


Figure 5.8 - GBE Factor interaction.

The risk detector computes the average values within ecosystems and determines if there are significant differences between the means of each stratum. Considering the country's extent, the mean value of GE corresponds to 51.47%. The mean value of BE referring to wetlands was 66.36% and 87.23% for freshwater ecosystems. All statistics were significantly different, considering a significant threshold of 0.05.

5.3.4. Inland GBE physical accounting: extent and condition

In 2018, forests, freshwater bodies, and wetlands covered around 62% of the territory of Continental Portugal. Forests occupied a total area of 5287284.95 hectares, freshwater bodies filled an area of 128391.01 ha, constituting roughly 1.7% of the total country area, and wetlands 0.33%, occupying an area of 21792.51 ha.

The condition of forests was assessed with the mean crown cover density (FCD), and the mean FWPI as a proxy for the status of freshwater and wetlands. The GBE status assessment is calculated by pixel, meaning that, in an area of 100 square meters classified as forests, 51% of this area will account for aboveground biomass. In a pixel classified as freshwater and wetlands, respectively, 87% and 66% will effectively account for Blue Ecosystems. The area (hectares), proportional extent (%), status (%), and physical accounts (%) of forests, freshwater bodies and wetlands in 2018 at the national scale are presented in Table 5.5.

Table 5.5 - Accounting for inland GBE extent and condition for Mainland Portugal in 2018.

Year 2018	Forest	Freshwater	Wetlands
Area (ha)	5287285	128391.01	21792.51
Proportional Extent (%)	60.36	1.7	0.33
Status (%)	51	87	66
Physical accounts (%)	31.07	1.48	0.22

5.4. DISCUSSION

We proposed a novel methodology that relies on RE techniques to disassemble TCD and WWPI datasets from the Copernicus products portfolio and redesign and reproduce them introducing new data and methods to enhance usability. Besides, our study delivered a hands-on approach to estimating climate-driven stock accounts of forest, freshwater, and wetland ecosystems. The findings on the drivers of biomass density and water availability shed new light on the potential implications of land cover conversions and climate conditions on inland GBE. This information is critical, given that these ecosystems are biodiversity hotspots capable of supporting a wide range of livelihoods, and able to provide a variety of goods and services.

5.4.1. Cloud-based automated classification of inland GBE

Open-access geospatial data streams and open-source software have made frequent, large-scale, high-resolution land cover mapping a reality (Arruda et al., 2021). These recent breakthroughs in acquiring and processing big earth data have made large-scale, high-resolution land cover classifications more viable for a diverse range of user groups, companies, and academics (DeLancey et al., 2019a). GEE has evolved in recent years as an appealing high-performance computing platform for cloud-based processing of petabytes of earth data, offering computational capability for planetary-scale data processing, as well as the ability to apply well-known ML algorithms (Gorelick et al., 2017).

The separation between GE and BE was implemented primarily to test the significant improvements in the accuracy and utility of such analyses (Koma et al., 2021). The fundamental motivation for segregating GE and BE into distinct categories arises from their inherently disparate spectral characteristics. Vegetation, characterized by its chlorophyll content and unique reflectance properties, displays pronounced spectral features in the green and near-infrared regions (Gitelson et al., 2003). Conversely, water bodies, including wetlands, exhibit spectral absorption patterns in the same regions (Khalid et al., 2021). These distinctive spectral properties lay the foundation for specialized classification approaches.

The classification analysis has underscored the improvement in classification accuracy achieved through this separation. The Kappa coefficient in both classifications showed compelling results. This enhancement in accuracy is not merely an academic achievement but has practical implications for informed decision-making (Jagannathan & Divya, 2021). Beyond accuracy, the separation of GE and BE enables tailored analysis for specific applications. For instance, GE classification supports studies related to vegetation health, land-use planning, and forest management, while BE classification aids in monitoring water bodies, wetland conservation, and hydrological assessments (Kulawardhana, 2011).

The F1 scores, indicative of the models' robustness in correctly identifying GE and BE categories, further emphasize the advantages of this separation (Alem & Kumar, 2022). GE achieved an F1 score of 0.93, while BE classification surpassed an F1 score of 0.94. These high F1 scores underscore the models' ability to effectively distinguish between these two categories.

A stand-alone ML classification model for mapping GE and BE has significant implications for environmental assessment, empowering researchers to conduct focused analyses on ecosystems, and supporting decision-makers in crafting sustainable land management and conservation strategies (Chignell et al., 2018; Z. Yang et al., 2021). Furthermore, the outputs of these classification tasks, the FCM from GE mapping and FWM from the BE were utilized to delineate ecosystem assets and quantify physical measurements of inland GBE (United Nations et al., 2021).

5.4.2. From Reverse Engineering to satellite-based climate-driven models

There is an emerging trend involving using SEO data to quantify ecosystem structure and functional traits which serve as more accurate indicators of ES than simplistic cover-based proxies (Schirpke et al., 2023). Their combination with regression models contributes to a comprehensive understanding of the social-ecological processes influencing the provision of ES and yields reliable data and results (C. Ramirez-Reyes et al., 2019) and thereby, provide cost-effective data to supply ecological accounts (Vargas et al., 2019).

The WWPI and TCD have the potential to provide data to build ecological-economic accounts for GBE. Redesigning and reproducing these datasets focused on forest, freshwater and wetlands evidenced the interdependency of some ecosystem functions, such as biomass density, water yield and soil moisture water content, and climatic and topographic drivers, as shown by Mengist et al. (2021). Topography and climate are key elements in explaining changes in vegetation abundance at the local (i.e. pixel, plot, or parcel scale) and regional levels (Mpakairi et al., 2022c).

FCD predictions were better than FWPI when comparing the results of R-squared, regression errors and residuals. The independent variables considered in both models were topographic characteristics (SLOPE and DEM) and climatic factors (PREC, PET and AI). Using the same factors to estimate different but correlated phenomena, demonstrated the intrinsic relationships between aquatic and terrestrial ecosystems (Cantonati et al., 2020; Dwire et al., 2018; Hose et al., 2021; Huang et al., 2020; Kløve et al., 2014; Koit et al., 2021). The aboveground biomass density represented by FCD estimates varies spatially and temporally according to ecosystem types, altitude, latitude, climatic conditions, and water presence (Tabacchi et al., 2011). GE supports biodiversity and many livelihoods around lakes, perennial streams, and wetlands, which benefit from BE's water and nutrient availability (Harris, 1984). Mpakairi et al. (2022) have shown that the density of healthy trees decreased due to limited water and nutrient availability, with water presence driving about 40% of biological processes in forests.

Regarding the contribution of each variable to the models, all of them showed to be relevant, a part of SLOPE presenting very low importance to both predictions. DEM and PREC were the factors that most contributed to the FWPI model, followed by PET, AI, and SLOPE. For the FCD model, PET and AI contributed the most, followed by PREC, DEM, and SLOPE. The results are aligned with those presented in the studies of Crowther et al. (2015) and Madrigal-González et al. (2023), analysing the influence of

climatic and topographic conditions in assessing GBE. These findings expanded our understanding of nature stock drivers, landscape behaviours, and increasing accuracy in ecosystem accounts. Therefore, unleashing the capacity to analyze the status and conditions of GBE helps to execute integrated natural resource management.

The geographical detector analysis used to verify spatial stratified heterogeneity enriched the knowledge of the drivers of GE and BE. The factor detectors indicate that both response variables are stratified by the exploratory variables, with more evidence of stratification shown by PREC, PET and AI. DEM showed a higher association with the BE than the GE model. Lastly, the physical accounts of inland GBE were assessed using the EA methodological framework. The physical accounts offer means to understand how sustainable the production is through measurements of natural stocks and yields, providing baselines for the assessment of ecosystems' capacity to deliver goods and services (Keith et al., 2020). The national GBE extent account represented their magnitude in terms of area in hectares, while the GBE condition described their integrity and status (Czúcz et al., 2021). The aboveground biomass in the forest was measured by calculating the area classified as forest, and the mean estimated value of FCD was applied to assess GE condition. BE were evaluated by determining the extent of freshwater bodies and wetlands and the mean estimated values of FWPI for each ecosystem.

5.4.3. Implications for future research

There are various difficulties with reverse engineering, especially when it comes to digital products (Chikofsky & Cross II, 2002). Other issues outside understanding the dataset itself include determining how it was created when we have little or no access to inputs, intermediate outputs, or even the code, algorithms, and tools used in each task (Wood, 2009). Without clear documentation of the model architecture, hyperparameters, and training process, it may be difficult for others to reproduce the results or understand the model's behaviour, and how the model arrives at its predictions.

The transparency through reporting the entire ML pipeline, including data preprocessing, model architecture, hyperparameters, and evaluation metrics enables others to reproduce and validate the results and improve the robustness and reliability of ML models, leading to better accuracy and more trustworthy results. Additionally, continuous monitoring and updating of models as new data becomes available can help maintain their performance over time.

Nowadays, a wide range of technologies exists to aid in the forward/reverse engineering process, especially in the production of digital products. A good improvement would be to provide more information about these products' development and make version control available to the public. This practice helps in keeping track of dataset modifications, comparing several dataset versions, and revert to whichever previous version is required.

Future research would further take these products apart to continue improving functionality, introducing new data and testing algorithms, as well as replicating to other areas in the globe. Additionally, it would be interesting to explore other products developed by Copernicus, which comprises a wide variety of products, such as Soil Water Index, Imperviousness Density and Impervious Built-up, Dominant Leaf Type and Forest Type, Coastal Zones and Protected Areas. These datasets are valuable resources for a wide range of geospatial services and environmental analysis.

5.5. CONCLUSION

This research demonstrated the potential of the TCD and WWPI products provided by Copernicus as fundamental data for ecological-economic studies and presented an approach to overcome limitations and enhance their usability. Besides, it underscores the significance of climatic (PREC, PET, AT) and topographic (DEM and SLOPE) variables influencing the status and conditions of GBE, by analyzing spatial relationships in the TCD and WWPI predictions. RE proved to be a valuable tool for innovation and problem-solving while examining the product's functionality and behaviour to determine how it works and identifying any vulnerabilities, weaknesses, or areas for improvement. The outcomes demonstrate the synergy of combining global open-access data with open-source technologies in creating predictive models that offer actionable insights, thereby facilitating evidence-based decision-making across various environmental and societal challenges.

6. REVEALING DYNAMICS OF CARBON STORAGE AND SEQUESTRATION IN FOREST ECOSYSTEMS: A DOWNSCALING APPROACH TO SUPPORT MONITORING PROGRESS TOWARDS SUSTAINABLE MANAGEMENT

6.1. INTRODUCTION

Carbon storage is one of many competing uses of land (Cunha et al., 2021). Globally, land use change and associated land management practices have always resulted in greater carbon inputs compared to the corresponding carbon sinks (Houghton et al., 2009). However, the conversion from forests to other land uses, primarily due to the increasing human population and urban sprawl, poses a particularly significant threat to forest carbon pools (Fitts et al., 2021). Carbon accounting studies play a crucial role in estimating the quantity of carbon sequestered over a period, providing useful insights for policymaking regarding human-environment interactions and future adaptive strategies (Nowak et al., 2022; Pan et al., 2023). These studies serve as proxies for assessing where certain land uses should be preserved to maintain their stores of carbon (G. Chen et al., 2020), as well as identifying locations where changes in land use can be implemented to minimize carbon emissions (Narine et al., 2019). Due to the correlation between carbon content and land use, there is a growing demand for precise mapping of carbon pools in many countries (Jiang et al., 2022), as land use patterns, in conjunction with the surrounding landscape, are crucial factors influencing carbon pool dynamics (Keith et al., 2021). This need is particularly emphasized by the Kyoto Protocol commitments (Tabacchi et al., 2011) and the sustainable development goals (SDG) proposed by the United Nations (Paganini et al., 2018). SDG 15 aims to preserve, restore, and encourage the sustainable utilization of terrestrial ecosystems, combat desertification, and address land degradation and biodiversity loss (United Nations, 2023). This urges countries to actively engage in forest conservation and promote sustainable forest management practices recommended to be implemented using Satellite Earth Observation (SEO) data combined with national inventories (Pan et al., 2023).

The SDG Indicator 15.2.1 allows countries to assess their progress, identify challenges, and implement effective strategies to manage forests sustainably, contributing to the achievement of environmental and socio-economic goals (Metternicht et al., 2020). This indicator is represented by measurements of forest area changes, forest health and vitality, biodiversity, and socio-economic benefits (United Nations, 2023). For instance, tracking changes over time in the total area covered by forests provided insight into deforestation, reforestation, and afforestation trends (Cao et al., 2022). Moreover, assessing the values and services provided by forest ecosystems such as the provisioning of wood and non-wood products, climate and water regulation, soil protection and recreational opportunities, ensures more protected forests and the preservation of biodiversity, while mitigating climate changes (Madrigal-González et al., 2023).

Cutting-edge technologies in remote sensing offer a time and cost-efficient method for estimating biophysical indicators of vegetation and surface conditions across wide temporal and spatial scales (J. Zhang et al., 2019). Applying SEO data and technologies makes it possible to build long-term observational records, facilitating the assessment of environmental changes over extended periods (Tyler et al., 2016). This allows the derivation of ecologically meaningful information that can be applied to large-scale monitoring applications (Holzwarth et al., 2020). The integration of satellite-derived products with change detection algorithms is one of the most promising approaches, holding

great potential for developing timely and accurate monitoring systems of natural resources (Reddy, 2021).

Estimating the amount of carbon in a landscape is crucial for several reasons (Seddon et al., 2021), particularly its impact on climate change and the assessment of forest health and productivity (Narine et al., 2019). Additionally, carbon stock accounts provide insight into the economic and social values derived from terrestrial ecosystems, such as the supply of benefits and services, opportunities for land use conversion, and the evaluation of carbon credits (Han et al., 2022). Opportunity cost refers to the value of the next best alternative forgone as a result of choosing one option over another (Golub et al., 2009). The analysis includes identifying land use options, evaluating direct and indirect benefits and costs, quantifying long-term and passive gains and comparing net present values. In the context of forest management, opportunity cost analysis is crucial for making informed decisions that balance ecological, economic, and social benefits (Navarro et al., 2017). This involves comparing the benefits of maintaining various types of forests with the potential gains from alternative land uses such as agriculture, urban development, or industrial activities (Costanza, 2020).

The InVEST Carbon Storage and Sequestration (CSS) model (Natural Capital Project, 2023) is an open-source software for modelling carbon storage and sequestration in terrestrial ecosystems. It provides information on the carbon content present in a landscape at a given point in time and the changes in carbon storage over time (Han et al., 2022). It is a tool to comprehensively evaluate the potential benefits of different land uses and management strategies in mitigating climate change and conserving carbon-rich ecosystems (Cong et al., 2023). There are a few research that used the InVEST CSS model to assess forest carbon pools. Islam et al. (2022) applied the InVEST CSS model in evaluating the carbon sequestration potential for different land use scenarios and highlighted the necessity of further research assessing carbon estimates for each terrestrial biome. Nawrocki et al. (2020) mapped species-level foliar cover addressing priorities of forest monitoring initiatives and emphasized the gap in new paradigms to map vegetation patterns at multiscale that better reflect observed variation and investigate the links between tree species and carbon sequestration. Fitts et al. (2021) modelled land use changes to estimate carbon stock in temperate forests in the United States and highlighted that future analysis must integrate remote sensing with other modelling approaches to assess the spatial extent of land use changes, and to understand the dynamics across forested landscapes.

In Portugal's mainland, forests are the most important natural resource, occupying around 34% of the territory (Eurostat, 2023). The most representative species are pine trees, cork and holm oak woods, and eucalyptus, providing a wide range of non-wood forest products such as cork, pinecone fruit and nut, and resin (FAO - UN, 2020). Every year, vast portions of the Portuguese forest are lost, due to fires, resulting in significant social, economic, and ecological impacts (Ermitão et al., 2023). This destructive phenomenon compromises public health, local communities, and industries dependent on forestry-related activities, while also disturbing the functioning of crucial ecosystem services, and releasing large amounts of carbon dioxide (CO₂) into the atmosphere.

To date, no research has been conducted focused on assessing multiscale forest carbon accounts, quantifying spatial patterns and the relationship between tree species and carbon stock, and mapping hot and cold spots of CSS in Mainland Portugal. Therefore, there are few related studies at the national level, such as Cunha et al. (2021) comparing different intervention scenarios of carbon sequestration and Fonseca et al. (2019) studying the impact of replacing tree species on carbon storage in a

mountainous area in the north of the country. The lack of research offering guidance on implementing multiscale carbon stock accounting leaves a gap in our understanding of opportunities for land use conversion based on the relationships between tree-species and carbon stock. Research outcomes enable the characterization of forest ecosystems in Portugal's mainland, serving multiple purposes such as biodiversity conservation, the implementation of sustainable management practices, and supporting policymakers in prioritizing present and future land use planning. The findings provide essential knowledge and important information on how carbon stock can be effectively assessed across different scales. Furthermore, at the national level, two of five SDG 15.2.1 sub-indicators were assessed: 1) the annual net change rate of forest area between 2018 and 2022, and 2) the estimation of AGB stored in the forest in the studied years. Measurement of these changes holds the potential to indicate the magnitude and distribution of carbon pools, support emissions inventories, and natural resources management, and enrich our knowledge of the carbon cycle, and the mechanisms responsible for governing terrestrial carbon sources and sinks.

To address these challenges, this study combines satellite data and technologies with forestry inventory to identify spatial patterns of AGB sequestered and stored in the national forest ecosystems. We present a methodology comprising a two-step classification model design to map forests at the tree-species level taking advantage of cloud computing capabilities provided by Google Earth Engine (GEE) (Google, 2022). The estimations of CSS are calculated using the InVEST CSS model, and the results are analysed using Exploratory Spatial Data Analysis (ESDA) tools in ArcGIS Pro (ESRI, 2023), such as Anselin's Local Moran's I statistic (Anselin, 1995), the Getis-Ord G_i^* statistic (Getis & Ord, 1992) and the Global Moran's I statistic (Moran, 1950). The outcomes are discussed across scales, starting at the national level, the analysis using NUTS III regions, and a finer-grained analysis encompassing the municipalities. This downscaling approach was needed to capture the spatial effects and patterns of CSS at regional and local scales of interest.

6.2. MATERIALS AND METHODS

6.2.1. Study area

The study area corresponds to mainland Portugal, which encompasses 90,000 km² of the Iberian Peninsula, located in southwestern Europe (Figure 6.1). The territory is divided into 23 NUTS (Nomenclature of territorial units for statistics) III subregions and 278 municipalities. The NUTS III classification is a hierarchical scheme designed to divide the economic territory of Europe into smaller geographical regions (Eurostat, 2023). The adoption of these analytical scales is suggested to harmonize human management considerations within the process of demarcation. However, it is essential to recognize that these choices can significantly influence the research findings and conclusions, due to spatial modelling to factors such as spatial granularity and scale (Turner et al., 1993).

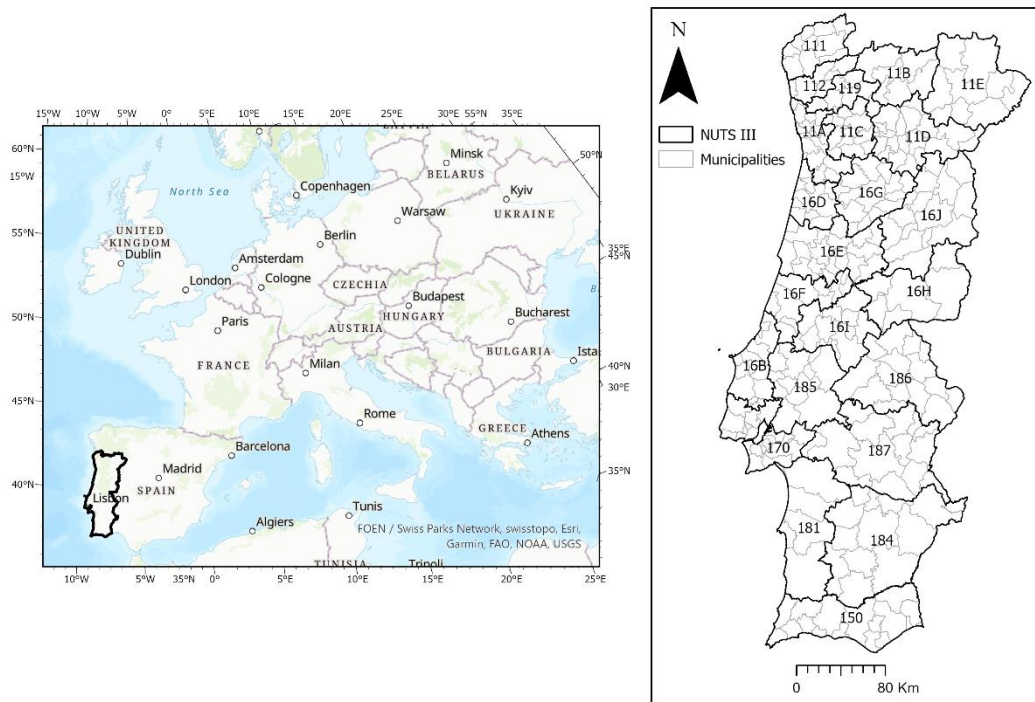


Figure 6.1 - Location of the study area.

The country's temperate climate reflects influences from both the Atlantic and Mediterranean regions, resulting in cold and wet winters and hot and dry summers (Coelho et al., 2013). The landscape is highly diverse, with the southern region of the country experiencing water scarcity and higher temperatures, resulting in less exuberant vegetation, contrasting with the more distinct Atlantic and Mediterranean climates found in the north (Almeida & Cabral, 2021). The flat terrain of the southern regions is associated with extensive agriculture and pastures in agro-forestry systems that feature low-density evergreen oak trees such as the Cork oak and Holm oak (Santos et al., 2023), while higher elevations in the central and northern regions are characterized by small landholdings, family agriculture, and forests of pine and eucalyptus. Asymmetries in human geography are also evident, with significant human presence and large settlements primarily concentrated along the coast, particularly from the capital city of Lisbon and extending northward (Araya & Cabral, 2010).

6.2.2. Data acquisition and processing

Sentinel-2 imagery, encompassing the entire mainland of Portugal for the years 2018 and 2022, was accessed through the GEE platform. All available spectral bands from Sentinel-2 imagery were used in data stacks, along with satellite-derived indices and topographic characteristics.

The spectral indices employed included the Normalized Difference Vegetation Index (NDVI) (Rouse et al., 1973) and Enhanced Vegetation Index (EVI) (Huete et al., 1997), used to highlight and distinguish vegetation of different types and at different stages of its evolutionary seasonal cycle. Additionally, the Soil Adjusted Vegetation Index (SAVI) (Huete, 1988) was utilized to reduce the impact of soil reflectance and enhance vegetation response. The topographic characteristics including slope and

elevation were derived from the Global Digital Surface Model dataset - Advanced Land Observing Satellite-3 (ALOS-3) with a horizontal resolution of approximately 30-meter mesh, provided by Japan Aerospace Exploration Agency (JAXA, 2023) free of charge.

To enhance the accuracy of the classification process, auxiliary data in the form of a set of reference polygons representing forest classes was also employed. These reference polygons were derived from the Portuguese land use and land cover map for the year 2018 (COS2018), developed by the Directorate General for Territory (DGT, 2018), a national organization responsible for the environment and land administration. This dataset served as ground truth data for a stratified sampling approach.

Additionally, the values of carbon density of AGB in each forest class were compiled from the 6th Portuguese National Forestry Inventory (ICNF, 2023). This information is required as input data in the InVEST CSS Model. Table 6.1 presents the seven classes assessed, encompassing, both individual species and groups, of the most representative forest species in Portugal's mainland, and their respective carbon density in tons per hectare (t/ha).

Table 6.1 - Forest class description, and carbon density (ICNF, 2023).

Forest class	Description	Carbon density (t/ha)
Cork oak forests	Cork oak including trees in agroforestry systems and other non-forest areas.	89.65
Holm oak forests	Holm oak forest, including trees in agroforestry systems and other non-forest areas.	53.67
Eucalyptus forests	Forests where the dominant species is eucalyptus (<i>Eucalyptus</i> spp.).	83.55
Forests of other broad-leaved	Areas comprising broadleaf tree species, including chestnut tree, carob tree, acacias, and various oak species, excluding cork and holm oak.	175.08
Maritime pine forests	Forests where the dominant species is maritime pine (<i>Pinus pinaster</i>).	137.56
Stone pine forests	Forests where the dominant species is stone pine (<i>Pinus pinea</i>).	85.71
Forests of other coniferous	Forests are dominated by species of resinous trees that do not belong to the maritime pine class and stone pine.	147.73

6.2.3. Methods

The outlined methodology is summarized in the diagram chart presented in Figure 6.2.

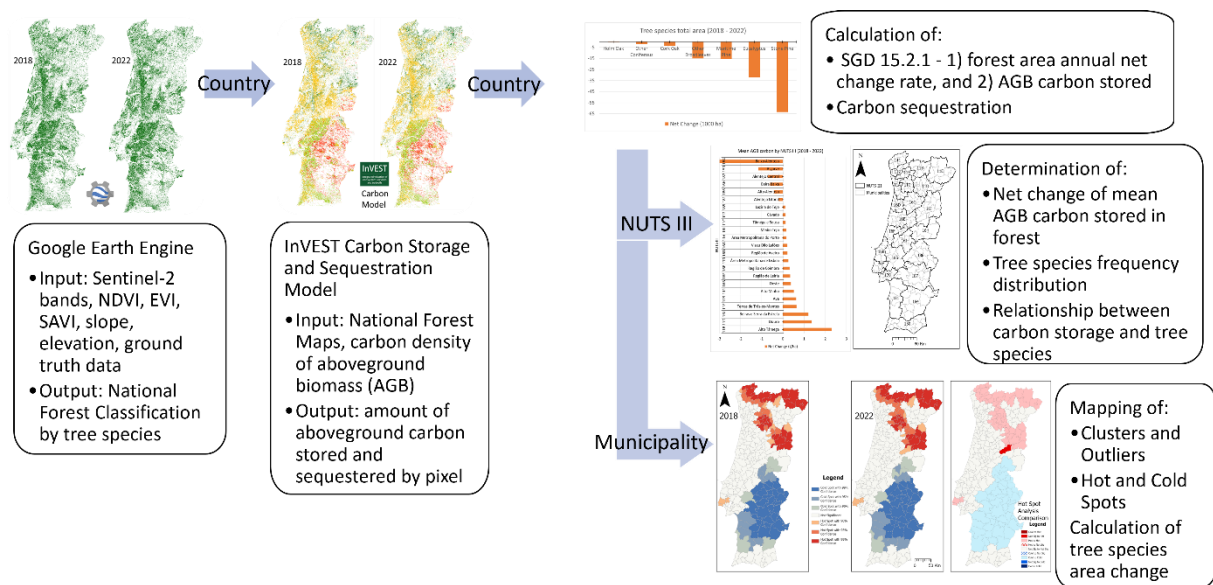


Figure 6.2 - Methodology schema.

The study relies on the GEE platform and its cloud processing and automated classifier capabilities to generate Portugal's annual forest mapping for 2018 and 2022, based on Sentinel-2 imagery, spectral indices, topographic characteristics and ground truth data. The modelling process starts with data acquisition and processing in GEE. The outputs were subsequently used as input data in the InVEST CSS Model to calculate carbon content sequestered and stored within the AGB of the forest at the country level, as well as the SDG 15.2.1 sub-indicators. Lastly, downscaling spatiotemporal analyses are performed using spatial statistics methods to determine the net change of mean AGB carbon stored and sequestered, tree species frequency distribution, the relationship between carbon storage and tree species, and to map clusters and outliers, hot and cold spots and calculate tree species area change.

6.2.3.1. National Forest Classification

Two classification tasks were applied to obtain the national forest species mapping. The outputs of the binary classification were utilized as masks in the subsequent phase. The first phase focused on binary classification, to map the presence or absence of forest class in each pixel (10m spatial resolution). In the second phase, multiclassification tasks were employed to detect seven different forest species classes, using all Sentinel-2 bands, spectral indices (NDVI, EVI and SAVI), and topographic characteristics (slope and elevation). By effectively filtering out non-forest areas in the first phase, the subsequent analysis would be better targeted, concentrating solely on the relevant features essential for accurate mapping. These specific species were identified within the forest pixels that had been recognized during the initial phase of the classification task and used the COS2018 dataset to define a total of 9800 reference points.

The Support Vector Machines (SVM) algorithm (Boser et al., 1992) was used in both classification tasks, binary (forest/non-forest) and multiclass (tree species). The utilization of the algorithm was based on its ability to handle complex datasets effectively and its well-documented success in distinguishing forest features (Ghosh, 2014; Grabska et al., 2020; Shao & Lunetta, 2012; Suess et al., 2015). Accuracy

assessments were carried out using a stratified random sampling protocol. The classification results were then subjected to an accuracy assessment procedure, encompassing the calculation of various metrics such as overall accuracy (OA), producer (PA), user accuracies (UA), and Kappa coefficient (K). OA is a class-independent accuracy metric and determines the general accuracy of an algorithm. The PA represents how well reference sample units are classified. Thus, the UA denotes the likelihood that a sample unit assigned to a certain class corresponds to that class in the ground. The Kappa coefficient is a statistical measurement of agreement often used as an overall measure of accuracy. The GEE scripts including all steps of classification tasks and the accuracy assessments are provided (A6. Appendix - Chapter 6, Table A6.1 and A6.2).

6.2.3.2. InVEST Carbon Model

The forest-tree species map outputs of the geospatial modelling in GEE served as inputs for the InVEST CSS model, enabling the estimation of carbon storage by forest classes and the amount of carbon sequestered during the period between 2018 and 2022. Carbon storage refers to the total amount of carbon accumulated within a carbon pool, whereas carbon sequestration is the process of capturing and storing CO₂ from the atmosphere. Sequestered carbon is the net amount of carbon captured and stored in a carbon sink over time. Our model only considers carbon values related to the AGB since the available data was limited to this pool.

As outputs, the CSS model generated comprehensive carbon storage raster maps for the study years, showcasing the amount of carbon sequestered and stored in each pixel. Positive values on the maps refer to carbon sequestration, representing the amount of carbon absorbed, while negative values indicate carbon loss, reflecting the amount of carbon released. These maps provide valuable insights into carbon dynamics, aiding in a better understanding of the ecosystem's carbon balance over time.

6.2.3.3. Spatial Patterns Analysis

Statistical tests are broadly categorized into global and local statistics, each offering unique insights into the distribution of spatial data and the detection of significant spatial trends (Ord & Getis, 2012). A global statistic was used to evaluate the presence of spatial clusters in the study area, employing the Global Moran's I statistic. This statistical measure tells us whether the pattern expressed is clustered, dispersed, or random. The associated z-scores and p-values enable us to understand the carbon stocks with low or high values clusters spatially. Moran's I index ranges from [-1, 1], where positive values indicate a positive spatial correlation. Larger positive values indicate a higher likelihood of spatial correlation, while negative values signify negative spatial correlation (Keith Ord & Getis, 2001).

After identifying the structure of global autocorrelation, a local statistic is used to detect the locations of clusters, such as Anselin's Local Moran's I statistic that detects clusters from the perspective of spatial autocorrelation, and the Getis-Ord Gi statistic employed to flag municipalities as hot and cold spots of carbon stocks. The flagging of local indicators of spatial association (LISA) is important to assess the influence of individual locations on the overall magnitude of the global statistic and to identify "outliers," mirroring the concept found in Anselin's Moran scatterplot (Anselin, 1995). It is worth noting that these results are only reliable when there are more than 30 features, making these tools well-suited for the municipality-level analysis, which counts 278 features.

The Anselin Local Moran's I (Cluster and Outlier Analysis) tool identifies statistically significant local clusters and spatial outliers (Tavares & Costa, 2021). A positive value for I indicates that a feature has neighbouring features with similarly high or low attribute values; this feature is part of a cluster. A negative value for I indicates that a feature has neighbouring features with dissimilar values; this feature is an outlier. In either instance, the p-value must be small enough for the cluster or outlier to be considered statistically significant, p-value smaller than 0.05 (95% confidence level). The tool requires setting up an appropriate spatial conceptualization of the phenomena, which will be chosen after trying inverse distance, inverse distance squared, fixed distance band, and k nearest neighbours.

Moran's Scatterplot provides insight into the extent to which individual pairs of values influence the global measure or may be interpreted as outliers, based on the extensive set of standard regression diagnostics. In the x-axis, the z-transformed is a vector with the observations (in deviations from the mean) and the y-axis represents the row-standardized spatial weights matrix W. It may be visualized as the slope of a linear regression of Wz on z . The four quadrants correspond to the four types of spatial association. The lower left and upper right quadrants indicate spatial clustering of similar values, and the upper left and lower right quadrants indicate spatial association of dissimilar values: low values surrounded by high neighbouring values for the former, and high values surrounded by low values for the latter.

The Hot Spot Analysis (Getis-Ord G_i^*) tool calculates the Getis-Ord G_i^* statistic value and both a z-score and p-value to evaluate the significance of that statistic. A high z-score and a small p-value for a feature indicate a spatial clustering of high values. A low negative z-score and a small p-value indicate a spatial clustering of low values. The higher (or lower) the z-score, the stronger the clustering effect. A z-score near zero indicates no apparent spatial clustering. Enabling the option of False Discovery Rate (FDR) correction guarantees that statistical significance is based on the p-value and z-score fields. The use of the FDR correction parameter is highly recommended so that critical p-values determining confidence levels are reduced to account for multiple testing and spatial dependence. For the Getis-Ord G_i , a positive value indicates a spatial clustering of high values (hot spot), and a negative value a spatial clustering of low values (cold spot).

6.3. RESULTS

6.3.1. National Forest Mapping

As for the accuracy assessment, results for the classification of forest species in 2018 and 2022 provide valuable insights into the classifier's performance (Table 6.2). In 2018, the OA stood at 91.01%, with PA at 88.61% and UA at 90.21%, resulting in a K coefficient of 0.88. Transitioning to 2022, the improvement in the classification performance is reflected in the results for OA (92.23%), while PA slightly decreased to 87.21%, UA to 89.85%, and K to 0.87. The GEE scripts for assessing classification accuracies are available (A6. Appendix - Chapter 6, Table A6.1 and A6.2).

Table 6.2. Comparison of forest classification accuracy (2018 vs. 2022) - Overall Accuracy (OA)%, User's Accuracy (UA)%, Producer's Accuracy (PA)%.

LULC	Overall accuracy (%)	Producers' accuracy (%)	Users' accuracy (%)	Kappa
2018	91.01	88.61	90.21	0.88
2022	92.23	87.21	89.85	0.87

6.3.2. Spatial effects on Carbon Storage and Sequestration

6.3.2.1. National level – Portugal Mainland

The two sub-indicators of the SGD 15.2.1 - 1) forest area annual net change rate, and 2) AGB carbon stored in the forest, are estimated at the national level, considering as reference years 2018 and 2022. Forest area change is determined by examining the value of the forest area change between reference years (Table 6.3). A negative value means forest loss, zero is no change, and a positive value means forest gain. In 2018 the total forest area on Portugal's mainland was 2711427 ha, in 2022 it was 2579482 ha. These estimations imply a reduction in the total forested area of 131945 ha and a loss change rate of around 32986.25 ha/year.

Table 6.3. Land Cover Changes and Dynamics of Forest Classes (2018-2022).

Forest class	Area (ha) 2018	Area (ha) 2022	Percentage 2018	Percentage 2022	Annual variation %
Cork oak forests	433231	429610	15.98	16.65	-0.21
Holm oak forests	437560	437390	16.14	16.96	-0.01
Eucalyptus forests	797594	765556	29.42	29.68	-1.00
Forests of other broad-leaved	437810	422818	16.15	16.39	-0.86
Maritime pine forests	448391	384968	16.54	14.92	-3.54
Stone pine forests	137233	121730	5.06	4.72	-2.82
Forests of other coniferous	19608	17410	0.72	0.67	-2.80
Total	2711427	2579482	100.00	100.00	-1.22

Consequently, the territory has reduced AGB stock which is also compromising the amount of carbon sequestered and stored. At the national level (between 2018 and 2022), Portugal decreased the amount of carbon captured by forest ecosystems by 0.22 t/ha (220 kg/ha). This biological carbon lost over time is due to a reduction in the AGB density represented by negative net changes in the forest's total area. The forest of Cork Oak exhibited a marginal decrease from 15.98% to 16.65%, accompanied

by a corresponding reduction in area measurements. Conversely, the Holm Oak class displayed a slight increase from 16.14% to 16.96%, with minimal changes in its spatial extent. The eucalyptus class, while experiencing an increase in annual percentage change, witnessed a notable change in its area from 2018 to 2022, with a reduction in the number of hectares. The forests of other Broad-leaved showcased a modest alteration from 16.15% to 16.39%, reflective of changes in the landscape composition. Notably, the Stone Pine and Maritime Pine classes both underwent considerable transformations, with Maritime Pine declining from 16.54% to 14.92% (accompanied by an annual change rate of -3.54%) and Stone Pine from 5.06% to 4.72% (with an annual change rate of -2.82%), each marked by substantial decreases in their spatial extent. The Other Coniferous class also demonstrated a marginal change from 0.72% to 0.67%, emphasizing the nuanced shifts in land cover dynamics, resulting in an annual variation of -2.80%.

6.3.2.2. Subregions - NUTS III

At the NUTS III level, Portugal sequestered a mean amount of carbon of 0.13 t/ha (130 kg/ha) by subregion, meaning that the mean AGB stock estimated by subregion increased by 32.5 kg/ha/year. The graphic (Figure 6.3) shows the net changes (t/ha) of the mean AGB carbon sequestered by forest ecosystems in each subregion. Subregions are identified also by the NUTS III code. Of 23, six subregions decreased the amount of carbon captured, while 17 sequestered carbon between the study years. The subregions that lost carbon over time are (184 - Baixo Alentejo, 150 - Algarve, 187 – Alentejo Central, 16H - Beira Baixa, 186 - Alto Alentejo, and 181 - Alentejo Litoral).

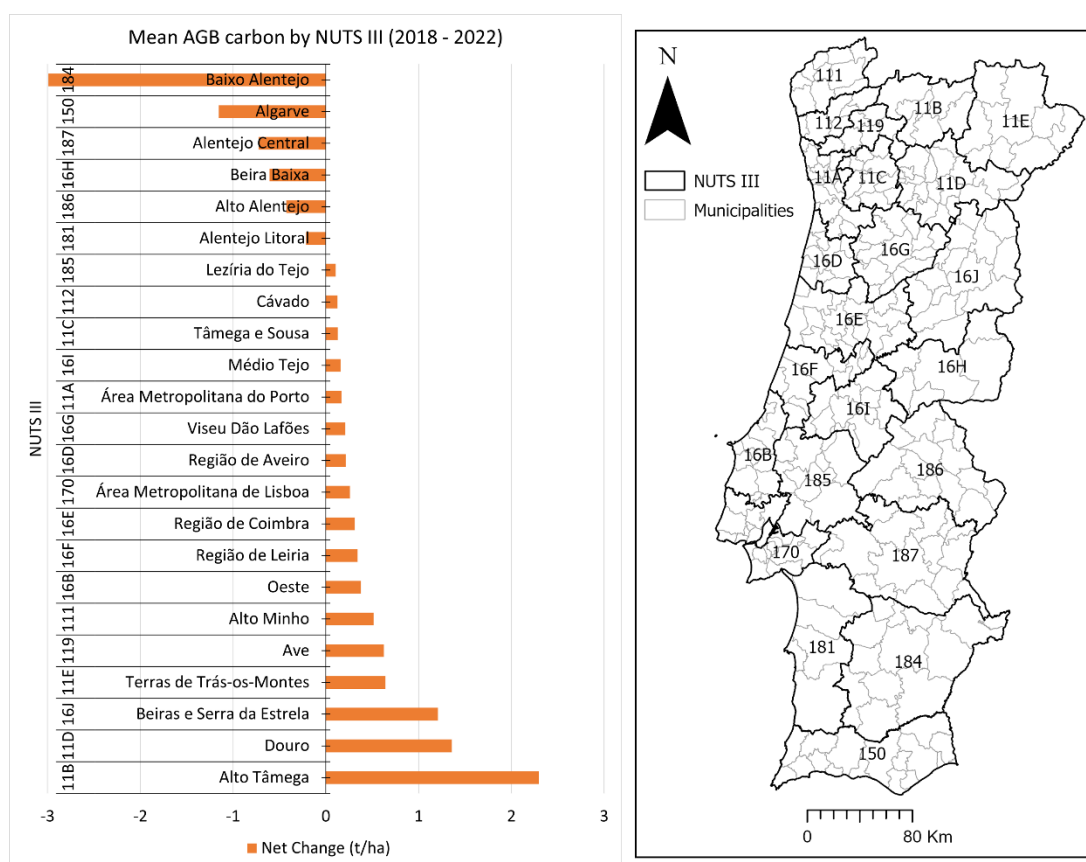


Figure 6.3 - Mean AGB carbon by NUTS III.

The amount of biological carbon captured and stored depends on the tree-species frequency distribution in each subregion (Figure 6.4). Comparing this information with the six flagged subregions that did not sequesterate carbon between 2018 and 2022, is possible to identify the species that most contributed to that loss.

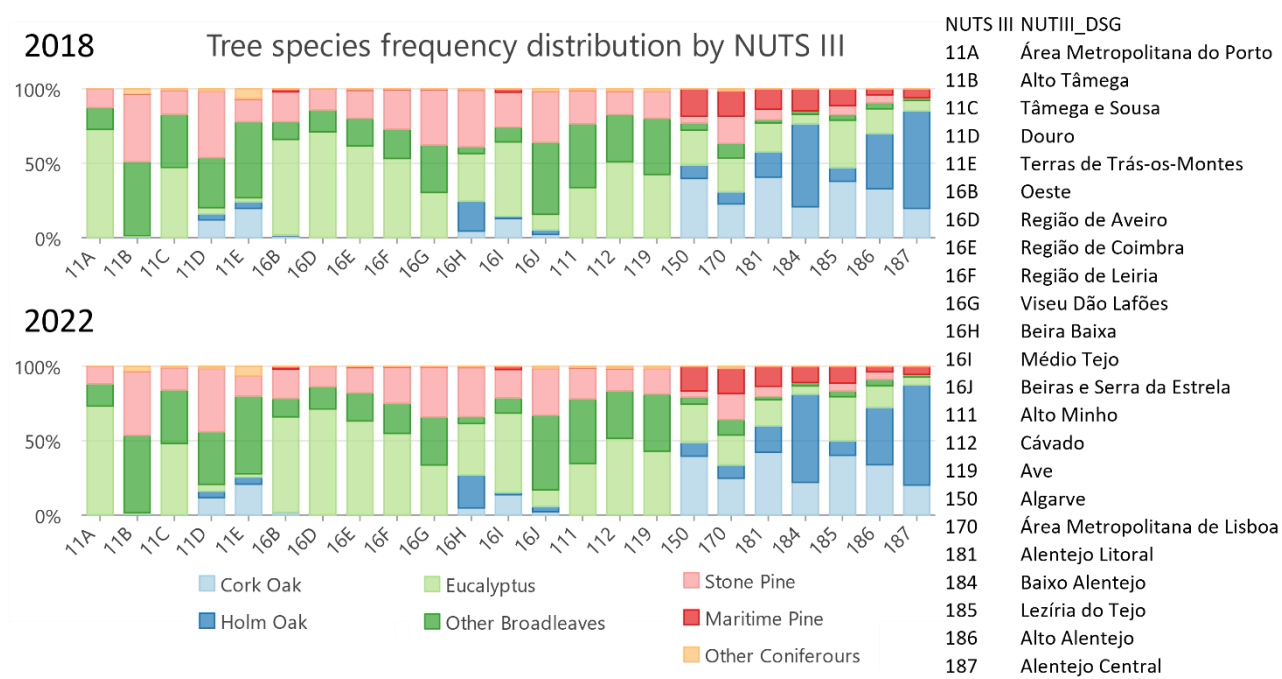


Figure 6.4 - Tree species frequency distribution by NUTS III.

In the graphics, we can see that the distribution of Stone Pine, Maritime Pine and Other Coniferous Forests decreased, and the Holm Oak increased in those six subregions. Other Broadleaves Forests increased in all subregions, except in 150 - Algarve and 181 - Alentejo Litoral. Eucalyptus Forests decreased in all subregions, except in the Algarve and 16H - Beira Baixa. To understand the relationship between the amount of carbon captured and stored and tree species at the NUTS III level, we estimated Pearson’s correlation for the studied years (Figure 6.5).



Figure 6.5 - Pearson's correlation for 2018 and 2022 of carbon storage and tree species.

The carbon storage shows a very high positive correlation with Other Broadleaves and a high positive correlation with Other Coniferous and Stone Pine Forests. A high negative correlation with Holm Oak, a negative correlation for Cork Oak and Maritime Pine and a low value for Eucalyptus. The relationship between carbon storage and tree species changed over time for Holm Oak, Eucalyptus, Stone Pine and Other Coniferous. Between 2018 and 2022 these associations increased for Holm Oak and Stone Pine and decreased for Eucalyptus and Other Coniferous. Within species, Cork Oak is well correlated with Maritime Pine Forests, as well as Other Broadleaves with Other Coniferous Forests.

6.3.2.3. Municipalities

The mean amount of carbon sequestered between 2018 and 2022, at the municipality level is 0.22 t/ha (220 kg/ha). The value of the Global Moran's I statistic is positive and statistically significant in both years (Table 6.4). These results mean that municipalities with high carbon storage in AGB forests correlate with high neighbouring values, and municipalities with low values correlate with low neighbouring values. The spatial autocorrelation is interpreted within the context of the null hypothesis which states that the AGB carbon storage is randomly distributed among the municipalities. Given that p-values are statistically significant, and z-score values are positive, there is less than a 1% likelihood that this clustered pattern could be the result of random chance, which rejects the null hypothesis.

Table 6.4. Global Moran's I statistic.

Year	Moran's Index	Expected Index	Variance	z-score	p-value
2018	0.6696	-0.0036	0.0007	23.8245	0
2022	0.6812	-0.0036	0.0007	24.234	0

These statistics were computed for a row-standardized spatial weights matrix based on k-nearest neighbours, given the importance of the neighbourhood in the study area. This conceptual spatial relationship ensures that each feature has a minimum number of eight neighbours in the analysis.

The first interpretation of local spatial patterns is diagnostic for outliers concerning a measure of global association. The I statistics are compared to the insights provided by the Moran scatterplot to visualize local instability in spatial autocorrelation. Figure 6.6 shows the distribution of significant positive (high-high and low-low clusters) and negative (high-low and low-high outliers) spatial autocorrelations for carbon storage in both years at the municipality level.

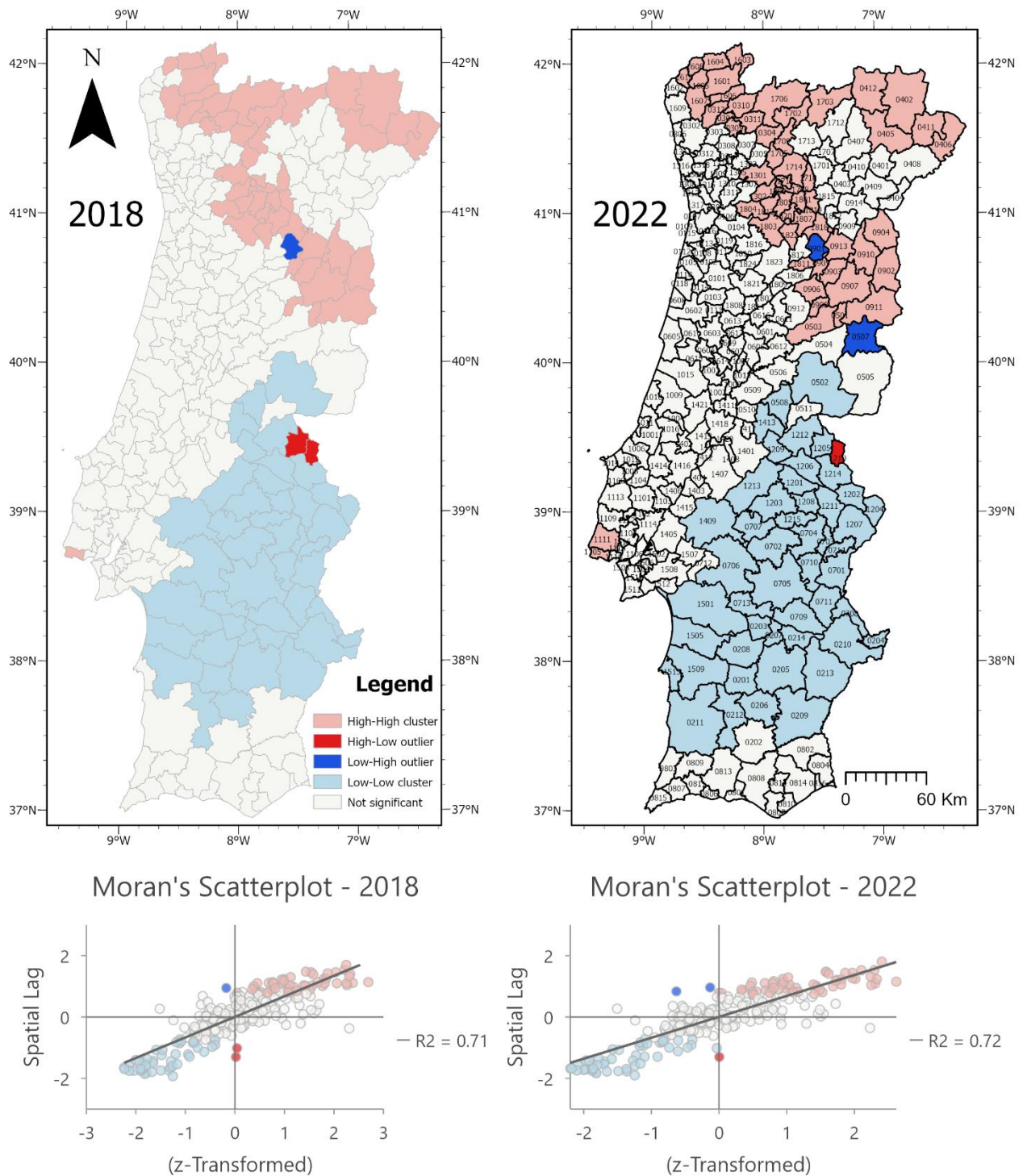


Figure 6.6 - Outliers and clusters distribution within studied years and Moran's scatterplots.

While the overall pattern of spatial association is positive, as indicated by the slope of the regression line (Moran's Scatterplots), in both years three observations show an association between dissimilar values. In the year 2018 is one in the upper left and two in the lower right quadrant. In 2022 are respectively two and one observations identified as outliers. Points in these quadrants indicate low

values surrounded by high neighbouring values for the former, and high values surrounded by low values for the latter.

Local Moran's I revealed local clusters of high–high values in 48 municipalities located in the northern of the country in 2018. Those are municipalities with high carbon storage surrounded by other high carbon storage areas. In this neighbourhood, one municipality was flagged as a low-high spatial outlier (0901 – Aguiar da Beira), where low values correlate with high neighbouring values. In the southern 44 municipalities were clustered by low-low values of carbon storage. Nearby were identified two municipalities with high-low values (1205 - Castelo de Vide and 1210 - Marvão). Of 278 municipalities, the results of 183 were not statistically significant, which means that we do not have enough evidence to reject the 'complete spatial randomness' hypothesis with 95% confidence.

In 2022 there are 56 municipalities clustered by high-high values in the northern of the country and another two with low-high values (0901 - Aguiar da Beira and 0507 - Penamacor). In the southern 48 municipalities are clustered by low-low values and one high-low outlier (1210 - Marvão). Of 278, the remaining 171 municipalities are not statistically significant.

Through the years 1205 - Castelo de Vide has changed from being a high-low spatial outlier to a low-low cluster, and Penamacor changed from not statistically significant to a low-high outlier. Odemira - 0211, Mértola – 0209, and Sines - 1513 have changed from not statistically significant to become a low-low cluster. Covilhã – 0503, Figueira de Castelo Rodrigo – 0904, Gouveia - 0906, Sintra – 1111, Vila Nova de Cerveira – 1610, Vila Real – 1714, Penalva do Castelo – 1811, and Paredes de Coura – 1605, have changed from not statistically significant to a high-high cluster.

The clustering phenomenon changing over time is detailed in Table 6.5. The mean values of carbon storage in the high-high clusters for both years were respectively 132.22 t/ha and 131.82 t/ha, and in the low-low clusters were 75.43 t/ha and 75.88 t/ha. In 2022, the mean value in the high-high cluster was lower, and the mean value in the low-low cluster was higher than in 2018. This statistical summary describes what has changed within clusters in the studied years.

Table 6.5. Descriptive statistics of carbon storage within clusters.

Year	Mean	Median	Standard Deviation	Variance	Minimum	Maximum	Count
2018	104.87	102.50	20.74	4.30	58.56	160.63	278
2022	105.09	102.64	21.49	4.62	57.94	161.32	278
2018_HH	132.22	130.07	13.74	1.89	105.83	160.63	48
2022_HH	131.82	129.03	14.45	2.09	105.15	161.32	56
2018_LL	75.43	74.42	10.64	1.13	58.56	96.60	44
2022_LL	75.88	75.78	11.65	1.36	57.94	104.39	48

The Getis–Ord Gi* statistic was used to identify the locations of statistically significant clusters with either high (hot spot) or low (cold spot) values. The results for each year and the hot spot analysis

comparison between years are presented in Figure 6.7. As in the Cluster and Outlier Analysis (Anselin Local Moran's I) tool, we use the k-nearest neighbour as the conceptual modelling for the spatial relationships.

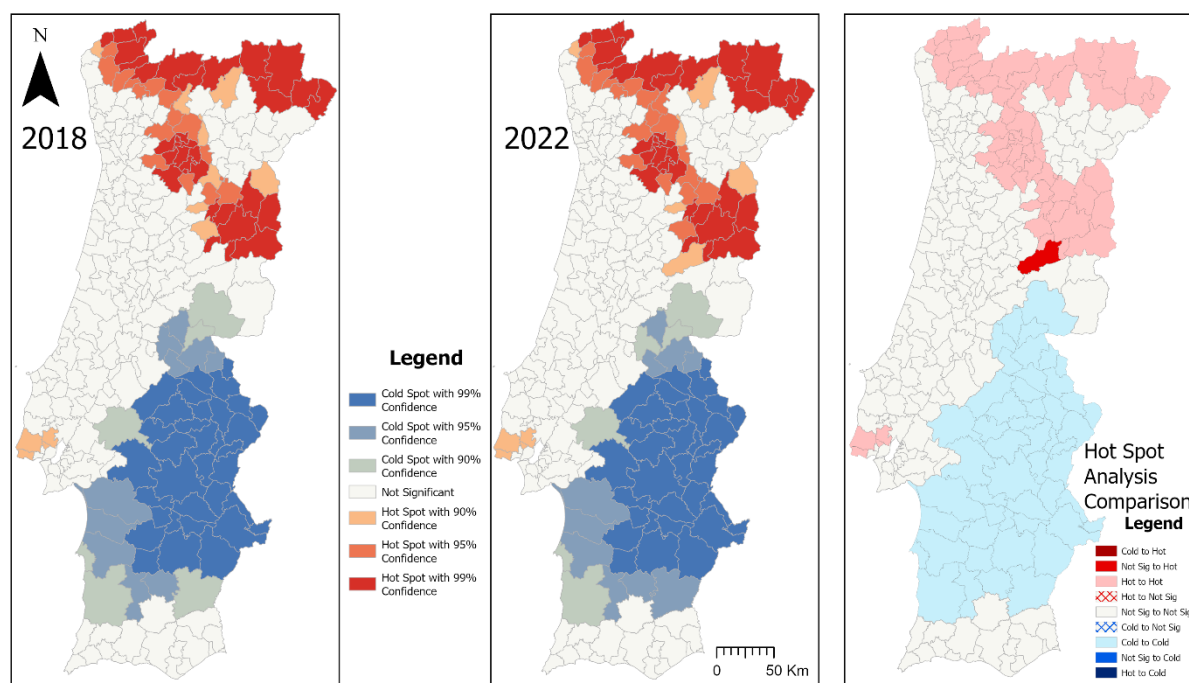


Figure 6.7 - Hotspot analysis comparison.

Results reveal the importance of inter-annual variations enabling the understanding of the forest ecosystem's functioning at the municipality level. At significance levels smaller than or equal to 10%, results show clusters (hot spot) with high carbon storage in the northern of the country and low (cold spot) in the southern. The north region displays hot spots of carbon storage in 59 and 60 municipalities, in 2018 and 2022, respectively. In the south, there were 50 cold spots, in both years. The maps highlight that six municipalities have changed through the years, increasing or decreasing their likelihood of being clustered as cold or hot spots when they do not. In the northern, Gouveia - 0906, Ribeira de Pena - 1709, and Sernancelhe - 1818 changed from hot 90% to hot 95%, increasing their probability of being clustered as hot spots. In the southern, Mértola – 0209 changed from cold 90% to cold 95% increasing their likelihood of being clustered as cold spots, and Mação - 1413, changed from cold 95% to cold 90%, decreasing their likelihood of standing out as cold spot. In the comparison analysis Covilhã - 0503 is highlighted, as the unique municipality that changed from not significant to hot 90%.

The graphic (Figure 6.8) depicts the changes between 2018 and 2022 in tree species areas in the flagged municipalities.

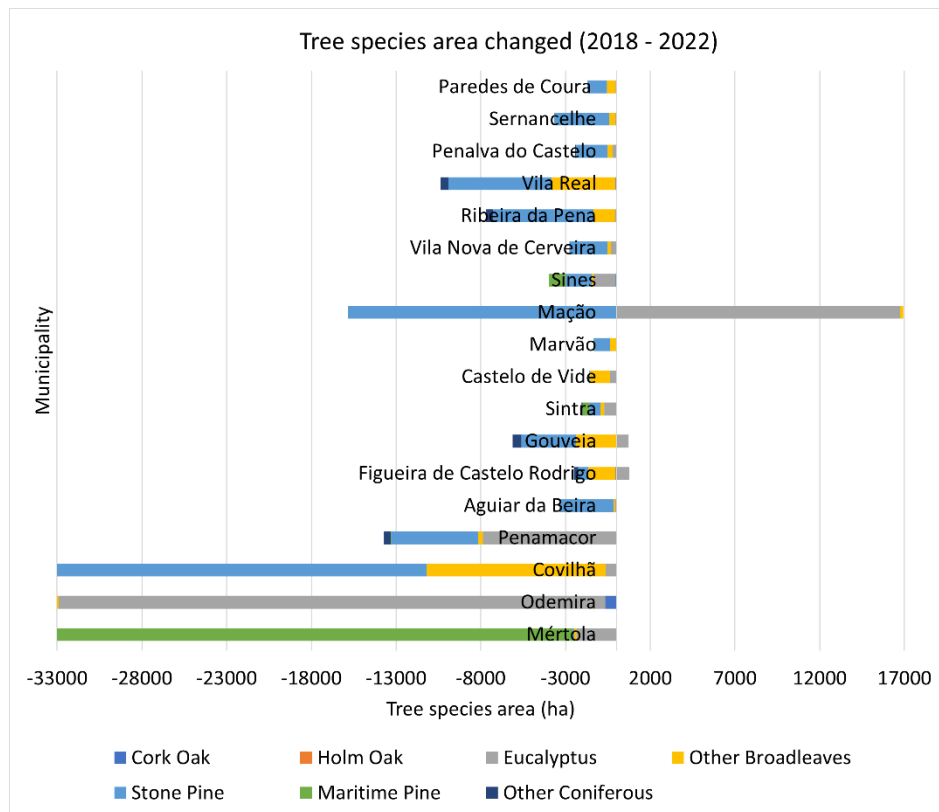


Figure 6.8 - Tree species area change in flagged municipalities.

Mértola possibly increased their likelihood of being clustered as cold spot because of a decrease in 31603 ha in Maritime Pine forests, while Mação decreased this likelihood, even losing 15822 ha of Stone Pine Forests area. This reduction in the level of significance of standing out as a cold spot can be due to an increase in the forest area of Eucalyptus (16726 ha) and Other Broadleaves (211 ha) that have the highest capacity of holding carbon. Covilhã is a unique municipality that has changed from not statistically significant to a hot spot cluster, even though it has lost 10566 and 25317 hectares of Other Broadleaves and Stone Pine Forests, respectively. Gouveia, Ribeira de Pena, and Sernancelhe increased their likelihood of being clustered as hot spots, even decreasing their forest area of Other Broadleaves and Stone Pine.

6.4. DISCUSSION

This study addresses the multiscale dynamics of CSS in forest ecosystems to support effective AGB carbon stock accounting and forest management practices. It contributes to better measurements of changes in carbon stock by developing an approach that takes advantage of cloud-based acquisition and processing of satellite data, the use of open-source software for modelling CSS, and the application of ESDA to study the relationship between AGB carbon storage and tree species, map clusters and outliers, and flag hot and cold spots of carbon storage at municipalities level.

6.4.1. Carbon stock accounting across multiple spatiotemporal scales

The multiscale analysis was important for understanding the spatial scale and granularity effects in modelling and assessing carbon pools. This investigation employed advanced spatial analysis and modelling techniques to address forest management issues and support enhancing forest carbon sequestration through strategic planning and management of land use. Most tools produce information at ranges that are too coarse for managers to understand and plan for (Gaur & Simonovic, 2019). The developed spatial downscaling approach adds value to the analysis and more accurate information to make well-informed decisions. The adoption of these methods was important for specific diagnoses and the development of strategies that can support solving environmental problems at the local level. While acknowledging the limitations of administrative boundaries, which may not always align with ecological scales, the use of administrative units remains necessary in studying socio-economic and environmental interdependencies and constructing spatially precise models. The results reveal the importance of analysing the inter-annual variations at the country, NUTS III and municipality levels. It advanced our understanding of the forest ecosystem's functioning and showed how the magnitude and distribution of AGB carbon density depend directly on vegetation species. Portugal reduced AGB stock in forest within studied years which had compromised the amount of carbon sequestered and stored. At the national level, the mainland territory decreased the amount of carbon captured by 0.22 t/ha (220 kg/ha). This biological carbon lost over time is due to a reduction in the AGB density represented by negative net changes in the forest's total area. Within forest species, the Stone Pine, Maritime Pine, and Other Coniferous classes marked the highest decreases in spatial extent, with annual % variations of -3.54, -2.82 and -2.80, respectively.

At the NUTS III level, Portugal sequestered a mean amount of carbon of 0.13 t/ha (130 kg/ha) by subregion, meaning that the mean AGB stock estimated by subregion increased by 32.5 kg/ha/year. Of 23 subregions, six decreased the amount of carbon captured, while 17 increased the mean AGB carbon sequestered within the studied years. The amount of biological carbon captured and stored was associated with the tree-species frequency distribution in each subregion. This fact was evidenced in the results of Pearson's correlation analysis with a high positive correlation between carbon storage and Other Broadleaves, Other Coniferous and Stone Pine forests, and high negative correlations with Holm Oak, Cork Oak and Maritime Pine with relationships also changing over time. Within species, Cork Oak was well correlated with Maritime Pine Forests, as well as Other Broadleaves with Other Coniferous Forests.

The mean amount of carbon sequestered between 2018 and 2022 at the municipality level was 0.22 t/ha (220 kg/ha), and the mean values of carbon stock in the high-high clusters for both years were respectively 132.22 t/ha and 131.82 t/ha, and in the low-low clusters were 75.43 t/ha and 75.88 t/ha. The Local Moran's I statistics for 2018 revealed local clusters of high-high values (hotspots) in 48 municipalities located in the northern of the country, while in the southern 44 municipalities were clustered by low-low values (coldspots). Unlikely, in 2022 there were 56 municipalities clustered by high-high values in the northern of the country and 48 municipalities in the southern. The local pattern analysis showed that over time eight municipalities located in the northern sector had increased their capacity to stock and sequester carbon, conversely, four municipalities located in the south of Portugal had decreased their capacity. These high spatial patterns of AGB carbon stock can be interpreted considering the climatic and topographic variability that characterize and divide the country into these two major regions (northern and southern).

6.4.2. Forest ecosystem mapping relied on satellite earth observation data and technologies

The integration of GEE-derived forest species maps with the InVEST CSS model offered a robust framework for estimating and visualizing CSS in forest ecosystems. The resulting maps not only highlighted the carbon dynamics but also served as crucial tools for informed decision-making in forest conservation and climate change mitigation strategies. However, detailed forest-cover mapping on a broad scale using supervised classification is technically constrained by many factors. Particularly, in our study's context of utilizing the SVM algorithm, significant challenges arise when aiming to accurately distinguish forest classes with comparable spectral signatures. The subtle intricacies of these spectral similarities can introduce confusion and misclassification, thereby affecting the accuracy of classification metrics (Sannigrahi, Chakraborti, et al., 2019a). Additionally, it is important to note that the effectiveness of the SVM algorithm relies on how we choose its parameters (X. Wang et al., 2021), which might not have fully encapsulated the inherent complexity of the data. Further adding to the intricacies are variations in sensor capabilities, atmospheric conditions, and temporal changes, which contribute to the uncertainty within accuracy assessments (Khwarahm, 2021). Despite these inherent limitations, the study underscores the robustness of SVM for forest ecosystem mapping. The classification performances were reflected in the results of OA with values larger than 91%, PA larger than 87%, UA higher than 89% and 0.87 for the Kappa coefficient.

To address the complexities introduced by closely related spectral signatures, future research endeavours could delve into integrating advanced techniques and comprehensive data sources. These measures, coupled with nuanced methodologies, hold the potential to mitigate limitations and enhance the accuracy of forest species mapping on a larger scale. The use of the grey-level co-occurrence matrix (GLCM) algorithm with satellite-derived indices would be further explored to capture forest structure, such as canopy height, and vegetation heterogeneity. As well as including other variables as predictors such as the leaf area index and the leaf Chlorophyll content to estimate canopy-leaf functional diversity. The introduction of these measurements will enable to capture of vegetation functional diversity and estimate of photosynthetic capacity and resource strategy of plants.

6.4.3. Monitoring progress towards sustainable forest management

Monitoring and managing carbon pools are integral parts of global efforts to address climate change and promote environmental sustainability (Keith et al., 2021). The two sub-indicators of the SGD 15.2.1 - 1) forest area annual net change rate, and 2) forest AGB carbon stock, were estimated at the national level, considering as reference years 2018 and 2022. In 2018 the total forest area on Portugal's mainland was 2711427 ha, in 2022 it was 2579482 ha. These estimations imply a reduction in the total forested area of 131945 ha and a loss change rate of around 32986.25 ha/year. Comparing these results at the national level with those from the Forest Resources Assessment – FRA 2020 for the year 2018 presented at the same scale (FAO - UN, 2020), our estimations of forest total area seem to underestimate the area corresponding to 6.8% of the territory (6125,70 km²). The same comparison is not possible for the year 2022, as it has not yet been provided by FAO. Cunha et al. (2021) also observed an underestimation in their calculations when analysing intervention scenarios using the InVEST Carbon Model. Their research pointed out the limitation of the CSS model in simplifying the earth's carbon cycle and assuming a linear change in carbon storage over time. Furthermore, the

outputs are only as detailed and reliable as the ground truth data and the AGB carbon density values used as a reference, added to the intrinsic limitations of the CSS model, such as not considering topographic and climatic variables, the presence of protected areas, and the age of trees. However, to overcome some of these flaws constrained by the CSS model, elevation and slope were included in the classification tasks.

The SDG Indicator 15.2.1 captures various aspects of sustainable forest management, reflecting the health, vitality, and benefits of forests (Estoque, 2020). The measurements of forest condition through carbon stock, species richness and habitat diversity, reflected forest degradation status, variety and abundance of species, and forest resilience in supporting various species and ecological processes. These assessments support monitoring national progress towards achieving sustainable forest management and allowing the comparison of progress with other countries and regions. Besides it provides data to inform policymakers with evidence-based decisions for strategic planning and management of land use and forest conservation.

The integration of forest management objectives into broader land use and development policies supports better land use decision-making based on the values gained at long-term and passive gains (Costanza, 2020). An opportunity cost analysis within forest types is a valuable tool to evaluate trade-offs, as the results showed different species have varying capacities for carbon sequestration. The benefits and costs can be represented by the provisioning capacity of supplying derived products such as timber, resins and nuts, or related services such as water and climate regulation, soil protection, and biodiversity conservation. Thus, have to include economic evaluations of goods and services associated with each forest-type option to compare alternatives. The methodology developed supports carbon accounts providing a systematic and thorough record of carbon stored and sequestered and can be applied at any other pools. Moreover, it helps to answer questions related to 1) the current distribution and quantity of carbon stored and/or sequestered in a landscape within a country, catchment, municipality or land parcel; 2) the carbon opportunity cost of land conversions; 3) mapping carbon sinks and sources; 4) identification of economic and social values provided by forest ecosystems.

6.4.4. Recommendations for enhancing forest carbon sequestration

A prioritised land use management can enhance CSS in forest ecosystems. Understanding the dynamics of carbon sequestration over time is critical for developing effective strategies to mitigate climate change and sustainably manage ecosystems, and determining carbon opportunity costs within tree species. These outcomes are important tools for environment protection, nature conservation, resource management, policymaking, and land use and landscape planning. This information may engage the general society by emphasizing the necessity of sustainable natural resource management, in addition to providing policymakers with the knowledge to overcome environmental challenges and make better decisions.

There are several recommendations and practices for helping countries mitigate climate change and achieve SDG. For instance, afforestation and reforestation focused on planting native, diverse and climate-resilient species, agroforestry practices integrating trees into agricultural landscape, restoration of degraded forests bolstering soil health through the application of organic amendments,

and water and erosion regulation, and invasive species control. Thus, protecting existing forests from deforestation and degradation is required to maintain their carbon storage capacity and enhance their resilience to climate change and other stressors. An adaptive management strategy anticipates and responds to changing climate conditions, including wildfires, and pest and disease control. As well as, establish protection efforts for vulnerable ecosystems, develop and implement policies to prevent illegal logging and land conversion, and engage local communities, providing them with incentives and alternative livelihoods. Continuous carbon stock monitoring systems and fluxes in forests using SEO and ground-based measurements are essential to understanding the carbon dynamics of different forest types and management practices. Furthermore, policies and incentives such as carbon credits, subsidies and grants must be developed and promoted to encourage land owners and stakeholders to adopt measures that optimize forest CSS.

6.5. CONCLUSION

Based on SEO data products, this study used geospatial technologies to analyse the forest carbon storage and changes in Portugal. Through multiscale spatiotemporal analysis, this study reveals the spatial heterogeneity of the carbon stock of seven forest types, which is of great significance for Portugal to rationally develop its carbon resources. This study offers a comprehensive methodology to assess the spatial effects and variability of carbon quantities, contributing to scientific knowledge and showing practical implications for forest management, carbon credit assessment, and climate change mitigation efforts. The main outcomes include baselines for implementing multiscale AGB carbon accounts to guide land use conversions through understanding the relationships between forest species and carbon stock. Besides, the downscale approach evidenced that the granularity of analysis is an important factor to be considered, especially for regional or local planning purposes.

7. CONCLUSIONS

7.1. SUMMARY OF FINDINGS

The outcomes of Stage 1 contributed significantly to the current understanding of the applicability of satellite-based ML models in assessing GBE. This stage not only identifies relevant techniques and applications but also serves as a basis for advancing model implementation and development. Moreover, it laid the groundwork for future research avenues through the proof-of-concept stage.

Through the systematic literature review, this work explored the development of ML models for assessing ESi based on RS data from Sentinel-2 and Landsat satellites. Quantification of environmental stocks, such as carbon, water, food production, raw materials, and energy has shown to be relevant for ESi accounting, globally. The ES categories with more ML models and applications developed were regulating (with climate regulation), provisioning (with the provision of genetic resources and raw materials), and habitat (with habitat service providing maintenance of genetic diversity).

Measuring the effects of implementing classification and regression tasks together instead of a single application provided a better understanding of researchers' decisions and their applicability of implementing hybrid models. An understanding of the satellite-based ML modelling components such as SEO technologies, instruments, data integration, and type of analysis or assessments, is important for recognizing the potential of SEO open data and technologies in modelling ES. The primary result of this meta-analysis was to assess the overall feasibility of using hybrid models, which involve both classification and regression together.

Results show that there were no rules regarding the selection of ML tasks, algorithms, or evaluation metrics, but meta-analysis indicated the likelihood of applying classification and regression tasks, specifically when assessing climate regulation, habitat, and genetic resources. Assessing ESi based on a non-parametric model is the best decision when one follows a set of good practices and has well conceptualized the study's purposes. When choosing an algorithm just because it is trending or easier to implement, it is quite dangerous, because it can be effective in solving certain problems, but not for a specific problem and/or dataset. Before building ML models, it is essential to understand the algorithms' drawbacks and limitations, such as the lack of transparency for the user, or the power computing required. The low accuracy of models stems from inadequate training data, compounded by a lack of transparency in reporting model implementation. This lack of transparency contributes to the *black box* problem, making it challenging to decipher the reasoning behind the results. Nonetheless, learners can be transparent and repeatable, and algorithm development is calling for advances that better link inputs, outputs, and intermediary steps. One good practice is not only to generalize the applicability of models, but to test performances between models and learners, and monitor the results through evaluation metrics. RF was the most implemented algorithm, followed by SVM. Choosing an algorithm that fulfils the requirements for each model is quite challenging. Making use of tools that compare algorithms and models is a better option, as they also commonly offer various elements of data handling, processing, and performance evaluation.

Reviewed studies highlighted opportunities for leveraging SEO in ES assessments and stressed the need for addressing challenges through innovative funding and partnerships to enhance global ES assessments. Challenges related to variable and model accuracy, data accessibility, technology

availability, and ethical considerations were pointed out as topics that require attention to ensure inclusive and meaningful technology use. They also suggest that integrating different technologies, fostering transdisciplinary collaboration, and exploring advancements in related research fields could provide further insights into environmental research.

The knowledge built in stage 2 demonstrates the applicability and robustness of methods providing guidelines to replicate research at multiscale. Through feasibility studies and sensitivity analysis data and methods were compared and evaluated. The first output of this stage included a reference table with global geospatial data to support studies related to the spatial estimation of water availability at the European level with the possibility of being implemented multiscale, as it includes global open-access data. The comparison of models was important to build confidence in the selected predictors. The outcomes guide future research to make better use of the globally available data that can be used as predictors in data-driven GBE modelling. Also, to advance the knowledge of the datasets provided by CLSM at the European level. The developed framework requires more deployment tests, nevertheless, model deployment has shown overall good results and the capability of being used worldwide as a baseline for modelling freshwater ecosystems. Another outcome of stage 2 was the comparison between seasons to capture the effects of seasonal climate variation and relationships between GE and BE. In dry periods, forests, lakes and rivers, and wetlands tend to show water stress, but if they have access to water sources, such as groundwater, the impacts between seasons tend to be less. This study provided a deeper understanding of how these natural systems should be modelled considering the dynamics of land use and seasonal climate effects. The sensitivity analysis advanced the knowledge in applying DL models in complex landscapes using also commercial GIS tools and increased our understanding of models' behaviours and improved models' predictions. The sensitivity tests showed that the hyperparameter settings are key to building accurate models and maximizing the benefits of each technique. Features' importance evaluation demonstrated the novelty of applying satellite products with contextual data to empower the model's quality, but a comprehensive conceptualization of the problem is the starting point for modelling success. The findings agreed with previous research as vegetation uses groundwater more during the driest season of the year when alternative water sources become depleted and evapotranspiration demand increases. This research would increase our understanding of inland aquatic and terrestrial ecosystems, including better information on the magnitude of seasonal climate variations and the variables that are more relevant to detecting those changes. Advancements in the development of ecological modelling help to monitor ES, minimize anthropogenic impacts and build resilience in the governance of natural ecosystems.

The proof-of-concept findings provided guidelines for the development and implementation of climate-driven models to assess the GBE capacity provisioning considering TCD and WWPI as indicators of GBE condition, and to map hotspots of CSS in forest ecosystems across multiple scales. The methodology presented in Chapter 5 relies on RE techniques to disassemble TCD and WWPI datasets from the Copernicus products portfolio and redesign and reproduce them introducing new data and methods to enhance usability. Results show high accuracy when reproducing both Copernicus products, including global climatic and topographic datasets, as predictors. Besides, this study delivered a hands-on approach based on ecosystem physical accounts to assess the status and conditions of GBE through the FCD and FWPI estimations across the spatial distribution of forest, freshwater, and wetland ecosystems. The findings on the drivers of biomass density and water availability shed new light on the potential implications of land cover conversions and climate conditions on inland GBE. This information is critical, given that these ecosystems are biodiversity

hotspots capable of supporting a wide range of livelihoods, and able to provide a variety of goods and services. The investigation presented in Chapter 6 unveiled the spatial effects of CSS within forest ecosystems by utilizing SEO data and technologies, carbon modelling and geospatial analysis. Through modelling the characterization of forest ecosystems in Portugal's mainland, two of five SDG 15.2.1 sub-indicators were assessed: 1) the annual net change rate of forest area between 2018 and 2022, and 2) the estimation of AGB stored in the forest in the studied years. Additionally, the findings underscore the relevance of investigating different scales and geospatial analysis methods, including a downscaling approach, to effectively capture the spatial effects and patterns of CSS. The results bear implications for land management strategies, conservation initiatives, and assessments of carbon credits, providing guidelines for implementing multiscale physical accounts of carbon for further land use conversions and opportunity cost analysis.

7.2. LIMITATIONS, CONTRIBUTIONS, AND DIRECTIONS FOR FUTURE RESEARCH

Synthesizing the review of included studies through meta-analysis has enhanced our understanding of the SEO data model's applications in assessing ESi. However, potential biases in the review process may lead to underestimations or overestimations of conclusions. We acknowledge the limitation of focusing on English-language studies, excluding valuable research reported in Chinese, Spanish, or Portuguese. Biases may also arise from the decision to concentrate on studies utilizing Landsat (4, 5, 7, and 8) and/or Sentinel-2. Recognizing that other studies employing different remote sensing technologies exist, our methodology allows users to assess, replicate, or update our findings.

The outcomes of this review contribute valuable information to the scientific community, offering a better understanding of SEO data and technologies' use and the applicability of ML models for ESi assessment. As the assessment and monitoring of changes in GBE support sustainable development, the results are relevant for decision-makers at multiscale levels. The reviewed studies demonstrate the utility of ML models for spatial characterization, environmental monitoring, and detecting changes in ESi, emphasizing the latest approaches used globally.

This study reveals the synergy of combining global open-access data with open-source technologies for predictive modelling, providing actionable insights for evidence-based decision-making. Advances in SEO data and technologies play a pivotal role in addressing environmental and societal challenges. The outcomes guide future research in making better use of globally available data, especially for water modelling and understanding CLSM datasets at the European level.

The study's framework, though requiring further deployment tests, offers valuable tools for natural resource management, biodiversity assessment, and evidence-based decision-making. The classification of GBE by seasons adds value to the modelling process, contributing to environment protection, nature conservation, resource management, policymaking, and landscape planning.

In future studies, standardized methods and a conceptual framework for model replicability are recommended. Researchers should address gaps, including the analysis of predictors, the use of spectral indices, and handling increasing data volumes in GBE modelling. The utility of such models in governance, policymaking, and landscape planning also warrants further exploration. Research should focus on discriminating seasonal wetlands from flooded areas, addressing algorithm choices and suitable scales for modelling.

The developed framework, while requiring more deployment tests, presents opportunities for assessing GBE and natural resources across multiple scales. Future research should evaluate other ML algorithms, explore additional spectral indices, and landscape metrics, and test SEO data from missions such as GRACE (Gravity Recovery and Climate Experiment) and radar satellites. Exploring other Copernicus products adds value to Earth observation and environmental analysis at the European scale, promising avenues for further research and development.

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A2. APPENDIX - CHAPTER 2

Table A2.1 - List of all studies included in the review.

Selected Studies
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Table A2.2 - Selected studies grouped by ES category.

ES Category	Study
Provisioning	(Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Mugiraneza et al., 2019), (Sharma et al., 2018), (Leroux et al., 2020), (Nawrocki et al., 2020), (Hunter et al., 2020), (Mallinis et al., 2020), (Zhu et al., 2022), (Zaimes et al., 2019), (Han et al., 2022), (Matsala et al., 2020), (Gwal et al., 2020), (Islam et al., 2022), (Pipia et al., 2021) , (Hudak et al., 2020), (M. Zhang et al., 2019), (Narine et al., 2019), (Silveira et al., 2019), (Sanderman, Hengl, Fiske, Solvik, Adame, Benson, Bukoski, Carnell, Cifuentes-Jara, Donato, Spalding, et al., 2018), (Y. Wang et al., 2017), (N. Pastick et al., 2018), (Morell-Monzó et al., 2020), (Hoffmann et al., 2022), (Hauser et al., 2021).
Habitat/ Supporting	(L. Zhang et al., 2022), (X. Yang et al., 2021b), (DeLancey et al., 2019b), (X. Wang et al., 2021), (Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Zhu et al., 2022), (Pipia et al., 2021), (Mugiraneza et al., 2019), (Mpakairi et al., 2022d), (Cilek et al., 2022), (Y. Zhang et al., 2022), (Lobert et al., 2021), (Nzuza et al., 2021), (Hasan et al., 2021), (Guo et al., 2021), (Agrillo et al., 2021), (Tarantino et al., 2021), (Vidal-Macua et al., 2020b), (Koskikala et

	al., 2020), (Boutsoukis et al., 2019), (J. Zhang et al., 2019), (Zaimes et al., 2019), (N. Pastick et al., 2018).
Regulating	(Mouta et al., 2021), (Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Mugiraneza et al., 2019), (N. J. Pastick et al., 2015), (Guio Blanco et al., 2018a), (Osborne & Alvares-Sanches, 2019a), (Fitts et al., 2021), (Wall et al., 2021), (Arruda et al., 2021), (Kundu et al., 2022), (Zormpas et al., 2017).
Cultural	(Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Osborne & Alvares-Sanches, 2019a), (Mugiraneza et al., 2019).

Table A2.3 - Studies grouped by ML algorithm.

Algorithm	Acronym	Study
Classification and Regression Trees	CART	(Pizarro et al., 2022), (N. J. Pastick et al., 2015), (Cilek et al., 2022), (N. Pastick et al., 2018), (L. Zhang et al., 2022), (Osborne & Alvares-Sanches, 2019a), (Mouta et al., 2021), (Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b).
Support vector machines	SVM	(Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Pizarro et al., 2022), (L. Zhang et al., 2022), (Kundu et al., 2022), (Y. Zhang et al., 2022), (X. Yang et al., 2021b), (Tarantino et al., 2021), (Mugiraneza et al., 2019), (Sharma et al., 2018), (Hunter et al., 2020), (Boutsoukis et al., 2019), (X. Wang et al., 2021), (Zhu et al., 2022), (Hauser et al., 2021), (Mouta et al., 2021).
Random Forest	RF	(Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Mouta et al., 2021), (Mpakairi et al., 2022d), (Han et al., 2022), (Fitts et al., 2021), (Wall et al., 2021), (Agrillo et al., 2021), (Matsala et al., 2020), (Morell-Monzó et al., 2020), (Koskikala et al., 2020), (Pizarro et al., 2022), (L. Zhang et al., 2022), (Hunter et al., 2020), (Boutsoukis et al., 2019), (Hudak et al., 2020), (Narine et al., 2019), (Nzuza et al., 2021), (Gwal et al., 2020), (Mallinis et al., 2020), (J. Zhang et al., 2019), (Nzuza et al., 2021), (Zaimes et al., 2019), (Silveira et al., 2019), (Sanderman, Hengl, Fiske, Solvik, Adame, Benson, Bukoski, Carnell, Cifuentes-Jara, Donato, Spalding, et al., 2018), (Guio Blanco et al., 2018a), (Y. Wang et al., 2017), (Mo et al., 2018), (Alqadhi et al., 2022), (M. Zhang et al., 2019).
Minimum Distance	MD	(Pizarro et al., 2022), (L. Zhang et al., 2022).
Deep Neural Networks	DNN	(Narine et al., 2019), (Hoffmann et al., 2022).
Maximum Likelihood Classification	MLC	(Cilek et al., 2022), (Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Islam et al., 2022), (Hasan et al., 2021), (M. Zhang et al., 2019), (Alqadhi et al., 2022).
Gradient Boosting	GB	(Nawrocki et al., 2020), (DeLancey et al., 2019b), (Mouta et al., 2021), (Osborne & Alvares-Sanches, 2019a), (Leroux et al., 2020), (Vidal-Macua et al., 2020b), (Nawrocki et al., 2020),

			(Matsala et al., 2020), (Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (N. Pastick et al., 2018).
CatBoost	CGB		(Ha et al., 2021).
Artificial Neural Network	ANN		(X. Wang et al., 2021), (Mouta et al., 2021), (Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b).
Naive Bayes	NB		(Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b),
Linear Discriminant Analysis	LDA		(Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b).
K-Nearest Neighbors	KNN		(Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Matsala et al., 2020), (X. Yang et al., 2021b).
Convolutional Neural Network	CNN		(Lobert et al., 2021), (Guo et al., 2021).
Multi-Layer Perceptrons	MLPN		(Arruda et al., 2021), (Alqadhi et al., 2022).
Gaussian Process Regression	GPR		(Pipia et al., 2021).
Linear Regression	LR		(Zormpas et al., 2017) (Mo et al., 2018), (Fitts et al., 2021).
Partial Least Square Regression	PLSR		(X. Wang et al., 2021).

Table A.2.4 - Studies that performed classification and regression tasks.

ML Task	Study
Classification and regression	(Sannigrahi, Joshi, et al., 2019), (Sannigrahi, Chakraborti, et al., 2019b), (Pizarro et al., 2022), (L. Zhang et al., 2022), (Kundu et al., 2022), (Y. Zhang et al., 2022), (X. Yang et al., 2021b), (Tarantino et al., 2021), (Mugiraneza et al., 2019), (Sharma et al., 2018), (Hunter et al., 2020), (Boutsoukis et al., 2019), (X. Wang et al., 2021), (Zhu et al., 2022), (Hauser et al., 2021), (Nawrocki et al., 2020)

A4. APPENDIX - CHAPTER 4

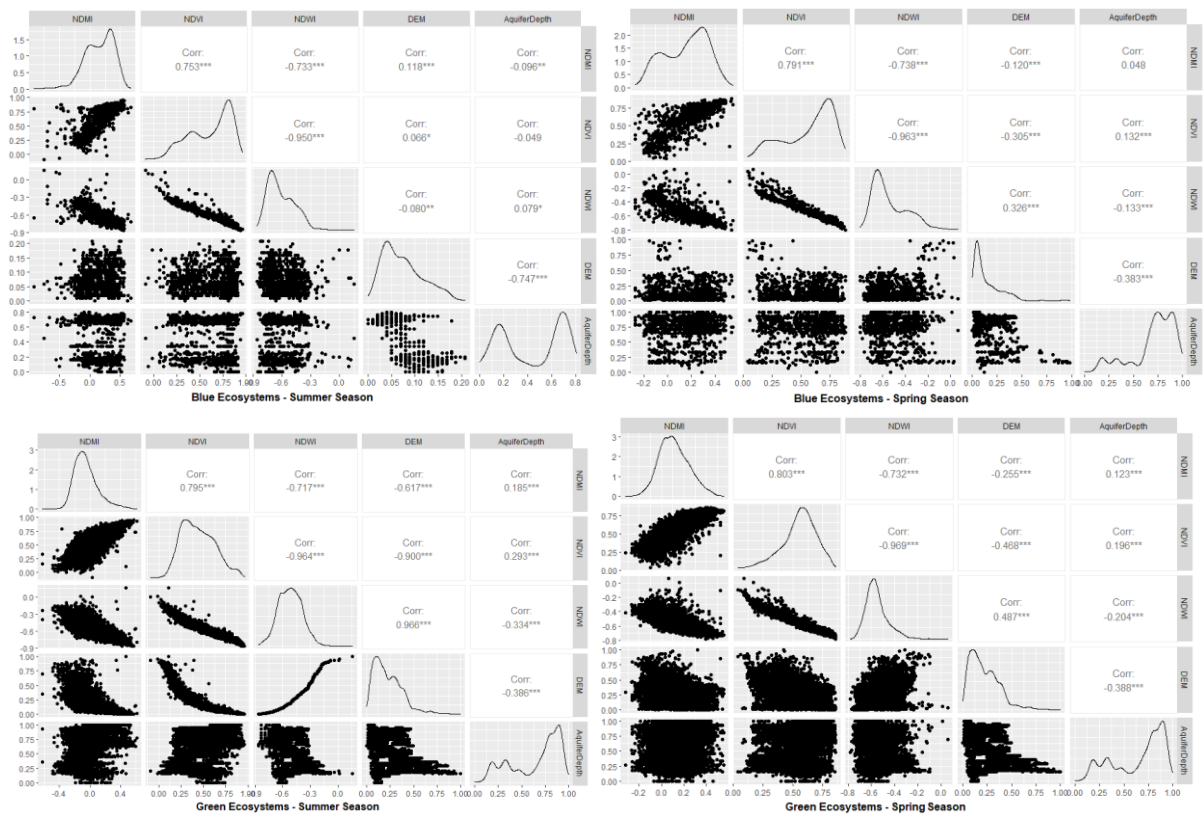


Figure A4.1 - Scatterplot matrix for each green and blue ecosystem by season.

A5. APPENDIX - CHAPTER 5

Table A5.1 - Spreadsheet of TCD and WWPI.

Characteristics	TCD	WWPI
	Tree Cover Density 2018 (raster 10 m), Europe, 3-yearly, Sep. 2020	Water and Wetness 2018 (raster 10 m), Europe, 3-yearly - version 2, Nov. 2020
Release/Major version	V2	V1, V2
Spatial coverage	Europe and the United Kingdom	Europe and the United Kingdom
Temporal extent	2018 (01/03/2018 – 31/10/2018)	2012-2018
Sensor	Sentinel-2A/2B	Sentinel-1, Sentinel-2A/2B
Thematic accuracy	>90%	Permanent water: 85%, Temporary water: 80%, Permanent wet areas: 80%, Temporary wet areas: 80%, Dry areas: 85%
Spatial resolution	10 m/100 m	10 m/100 m
Format	GeoTIFF (1.0)	GeoTIFF (1.0)
Spatial representation	Grid	Grid
Land Use Mask	Forest Cover (FAO)	(1) permanent water, (2) temporary water, (3) permanent wetness and (4) temporary wetness.

Scripts for binary classifications in Google Earth Engine.

Table A5.2 - Binary classification of forest ecosystems.

https://github.com/MASOTs/MapGBEonGEE/blob/main/classification%20_vegetationNonVegetation.txt

Table A5.3 - Binary classification of freshwater and wetland ecosystems.

https://github.com/MASOTs/MapGBEonGEE/blob/main/classification%20_waterWetlands.txt

A6. APPENDIX - CHAPTER 6

Scripts for binary and multiclass classifications in Google Earth Engine.

Table A6.1 - Binary classification of forest ecosystems.

https://github.com/MASOTs/MapGEonGEE/blob/main/classificacao1stPhase%20_foresNoForest.txt

Table A6.2 - Multiclass classification of forest ecosystems.

https://github.com/MASOTs/MapGEonGEE/blob/main/classificacao2ndPhase_forestSpecies.txt



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