Reviews and syntheses: Remotely sensed optical time series for monitoring vegetation productivity

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Abstract. Vegetation productivity is a critical indicator of global ecosystem health and is impacted by human activities and climate change. A wide range of optical sensing platforms, from ground-based to airborne and satellite, provide spatially continuous information on terrestrial vegetation status and functioning. As optical Earth observation (EO) data are usually routinely acquired, vegetation can be monitored repeatedly over time; reflecting seasonal
5   vegetation patterns and trends in vegetation productivity metrics. Such metrics include e.g., gross primary productivity, net primary productivity, biomass or yield. To summarize current knowledge, in this paper, we systematically reviewed time series (TS) literature for assessing state-of-the-art vegetation productivity monitoring approaches for different ecosystems based on optical remote sensing (RS) data. As the integration of solar-induced fluorescence (SIF) data in vegetation productivity processing chains has emerged as a promising source, we also include this
10   relatively recent sensor modality. We define three methodological categories to derive productivity metrics from remotely sensed TS of vegetation indices or quantitative traits: (i) trend analysis and anomaly detection, (ii) land surface phenology, and (iii) integration and assimilation of TS-derived metrics into statistical and process-based dynamic vegetation models (DVM). Although the majority of used TS data streams originate from data acquired from satellite platforms, TS data from aircraft and unoccupied aerial vehicles have found their way into productivity
15   monitoring studies. To facilitate processing, we provide a list of common toolboxes for inferring productivity metrics and information from TS data. We further discuss validation strategies of the RS-data derived productivity metrics: (1) using *in situ* measured data, such as yield, (2) sensor networks of distinct sensors, including spectroradiometers, flux towers, or phenological cameras, and (3) inter-comparison of different productivity metrics. Finally, we address current challenges and propose a conceptual framework for productivity metrics derivation, including fully integrated
20   DVMs and radiative transfer models here labelled as "Digital Twin". This novel framework meets the requirements of multiple ecosystems and enables both an improved understanding of vegetation temporal dynamics in response to climate and environmental drivers and enhances the accuracy of vegetation productivity monitoring.

1   Introduction

Vegetation productivity, the rate at which solar energy is converted into biomass through photosynthesis, is the
25   origin of all fuel, fiber, and food by which humanity and many other species live, and should therefore be closely

monitored. The total amount of photosynthesis on Earth defines the planetary boundary of production, which is a measure of how much of the planet's productivity humans have appropriated (Ryu et al., 2019). According to the United Nations (UN), the global population is expected to reach 9.7 billion by 2050; presenting a significant challenge for ensuring sufficient future food production. The productivity of plants is a crucial factor in meeting this challenge, as it directly affects the amount of food that can be produced. Plant productivity thus fundamentally delineates the habitability of our planet (Running et al., 2000).

The intensification and spatial expansion of human activities in recent centuries have profoundly altered the world's natural and cultural landscapes (Winkler et al., 2021), and have had a significant impact on ecosystem processes, and their functions in society. An integrative proxy of this global change is the altered regime of vegetation productivity. As a key characteristic of ecosystem conditions, global vegetation productivity reflects both, the spatial distribution and change of the vegetation coverage (EEA, 2021). The key climatic drivers of vegetation productivity are temperature, water supply and solar radiation (Madani et al., 2018), which interact to constrain the magnitude and temporal dynamics of ecosystem productivity depending on soil conditions. In the twenty-first century, it is expected that vegetation productivity will decrease due to the impacts of climate change in the Northern Hemisphere, and may negatively affect the global land carbon (C) sink with unknown feedback effects (Zhang et al., 2022b).

Due to variations in vegetation composition, climate, soil properties, and management practices among others, vegetation productivity is heterogeneous across space. In addition, this variation occurs at all timescales, from diurnal over seasonal to inter-annual. Thus, to achieve accurate global estimates of plant productivity that explicitly account for spatial and temporal variation, it is essential to acquire continuous spatial observations over time using optical Earth observation (EO) satellites. Remotely sensed time series (TS) from those EO data streams provide the basis for phenological monitoring, which is unequivocally related to productivity (e.g., Zhu et al., 2016). Phenological monitoring is the study of the timing of recurrent, annual biological events (e.g. budburst, flower blossoming, leaf senescence), and shifts in the timing of seasonal phenological events have been shown to be related to inter-annual variations in annual productivity (e.g., Park et al., 2019). Consequently, among the objectives of the EO satellite missions launched in the last five decades, primary importance has been given to observing the productivity and health of natural and cultivated vegetation land covers (e.g., Chevrel et al., 1981; Huete et al., 2002; Zhang et al., 2003; Atzberger, 2013). Novel satellite systems are launched constantly and significant improvements in data-driven, as well as physically based data analysis techniques are made (Baret and Buis, 2008).

These developments demand a systematic overview of the state-of-the-art TS studies related to vegetation productivity, presenting the unprecedented availability of continuous multi-sensor data streams, constantly updated data repositories, and the latest processing techniques and toolboxes. Recent review papers focused on global land surface phenology (LSP) research (Zeng et al., 2020; Caparros-Santiago et al., 2021), but lacked the relationship to vegetation productivity. Other reviews were restricted to specific ecosystems (Berra and Gaulton, 2021) or sensors (Eitel et al., 2016). Microwave-based studies were covered by Teubner et al. (2018); Wild et al. (2022).

Therefore, we formulate for this review the following main research question: **What are the state-of-the-art methods for estimating vegetation productivity using remotely sensed TS data streams, and what are the key gaps, challenges, and opportunities for further improvement?**

To address this question, our main emphasis is on the precise EO-based estimation of productivity with consideration of the trend towards the increasing availability of higher spatial resolution EO data. Global change is resulting in a landscape that is more fragmented, scattered, and characterized by small-scale patterns. One example is the upcoming trend of agroforestry to make agriculture more resilient. As a consequence, the analysis of productivity needs to integrate high-resolution EO data. Hence, we will focus on the literature that uses remotely sensed optical TS and derived proxies for quantifying productivity, with a greater emphasis on the spatial scale than on the minimum number of time steps.

The review is divided into seven sections, where Sect. 1 provides a tangible definition of productivity, and introduces the main productivity metrics and methods. Sect. 2 describes the available optical sensor platforms. Sect. 3 provides the methods in detail and toolboxes for processing, analysing, and modelling TS data streams. In Sect. 4 we outline three different strategies for validating productivity products. The outcomes of the systematic literature review are provided in Sect. 5. In Sect. 6 we provide an outlook on future challenges to assess vegetation productivity from TS data, followed by a conclusion (Sect. 7).

1.1 Definition of productivity adopted for this review

Productivity in ecosystems quantifies the rate at which autotrophic organisms, such as green plants, convert energy into organic metabolic assimilates (Scurlock and Olson, 2002; Larcher, 2003). Vegetation productivity is controlled by two processes; (i) the assimilation of CO_2 substrate through photosynthesis (source activity) and (ii) tissue growth from the accumulated carbohydrates into stored biomass (sink activity) (Körner, 2015). Plant photosynthesis is driven by incoming photosynthetic active radiation, CO_2 concentrations, temperature, and water and nutrient availability (e.g., Ryu et al., 2019).

Vegetation productivity is commonly defined in four measures: gross primary productivity (GPP), net primary productivity (NPP), net ecosystem productivity (NEP) and net biome productivity (NBP). The interplay of these main productivity measures is illustrated in Fig. 1.

Over small spatial extents ($< 1km^2$), NEP is usually directly estimated through eddy-covariance (EC) methods, where the vertical, turbulent fluxes of CO_2 are measured within the atmospheric boundary layer using CO_2 concentration measurements from an infrared gas analyzer (IRGA) along with high-frequency sonic anemometer wind velocity measurements. NEP is subsequently partitioned into GPP and ecosystem respiration (Re), where estimated Re values are commonly derived from nighttime fluxes (i.e. NEP = Re) when GPP is zero and extrapolated to daytime fluxes. The ratio of NPP to GPP is termed the carbon use efficiency and represents the capacity to which plants are able to transform assimilated CO_2 into stored biomass, after carbon losses through autotrophic respiration (Ra). The carbon use efficiency of vegetation varies according to factors such as plant species, nutrient availability,

light, temperature, and water availability. However, the ratio of NPP to GPP is typically thought to be around

95   0.45, according to empirical studies, satellite products and process-based models (He et al., 2018), indicating that 55% of the carbon captured by plants is directed towards respiration and thus cannot be utilized for net production and growth (Field et al., 1998). NBP is the net amount of carbon dioxide that is assimilated by an ecosystem over a period of time, after accounting for all losses of carbon dioxide through respiration, decomposition, and other processes. NBP is thus a measure of the overall health and productivity of an ecosystem, and it is an important

100 factor in the global carbon cycle. Input and losses of NBP are on a rather long time scale for natural landscapes and for agriculture it refers to harvest (e.g., Prescher et al., 2010; Turner et al., 2007).

Although NPP and GPP are common metrics to express the productivity of any ecosystem, in the literature different definitions or terms can be found. For instance, in agroecosystems, productivity often refers to aboveground (and below-ground) biomass (AGB) and yield (Chopping et al., 2011; Mariotto et al., 2013). In forestry, productivity

105 is also often related to AGB or harvestable wood (Battles, 2022). For natural ecosystems, AGB, (e.g., Ramoelo et al., 2015; Lumbierres et al., 2017) but also directly NPP and GPP are commonly used to express productivity (see e.g. reviews by Anav et al. 2015; Liao et al. 2023). In the current review, we refer to all these productivity metrics, which are summarized in the blue box.

Definitions of productivity metrics

Productivity is the rate at which a quantity (e.g., energy) is accumulated by producers (e.g., plants) over time within a given area. Here we give an overview of metrics for productivity adopted in our review:

- **Gross primary productivity (GPP)** is the total amount of C photosynthesized by plants (Myneni et al., 1995) in a given time (g C/m^2/day) and describes also the largest carbon flux between the biosphere and the atmosphere (approximately 130 Gt C per year) (Krause et al., 2022).

- **Net primary productivity (NPP)** denotes the remaining C from photosynthesis after respiration losses from plants (Ra) (g C/m^2/day), which is invested for the maintenance of cells and the growth of tissues (Roxburgh et al., 2005).

- **Net ecosystem productivity (NEP)** is defined as NPP minus soil heterotrophic respiration (Rh) by microorganisms (g C/m^2/day), i.e., C loss from the decomposition of woody detritus, soil organic matter, vegetation mortality, grazing, etc. (Landsberg and Gower, 1997). It reflects the temporal change in C that can be stored in an ecosystem (Harmon et al., 2011). NEP thus quantifies the loss or accumulation of C within an ecosystem and defines if it is acting as a sink or source of C.

- **Net biome productivity (NBP)** on a regional scale represents the net change in carbon within ecosystems. It is calculated by adjusting NEP for lateral carbon transfers to neighbouring biomes, which may occur through various processes such as harvest, organic matter export in rivers, or losses from disturbances such as wildfires (e.g., Schulze et al., 2021; Prescher et al., 2010).

- **Aboveground biomass (AGB)** is the total amount of plant matter on the soil surface in a given area or ecosystem that has accumulated over time, as a result of photosynthesis and plant metabolism (kg C/m^2). AGB plays a crucial role in quantifying the productivity of forests etc. as it specifies the amount of stored carbon per unit area and subsequently the capacity for water filtration, soil retention, and biodiversity conservation (Powell et al., 2010; Goetz et al., 2009).

- **Crop yield** is defined as the amount of the harvested product (e.g., kg grain) per unit cropped area (kg/ha), and is a measure of productivity referring to the part of biomass that can be used for the nutrition of humans, feeding of livestock, the production of fuel or construction materials (Carletto et al., 2015).

- **Harvestable wood** refers to productivity in forests, typically given in cubic meters of harvestable wood grown per year on a forested site (m^3/ha) (FAO, 2010).

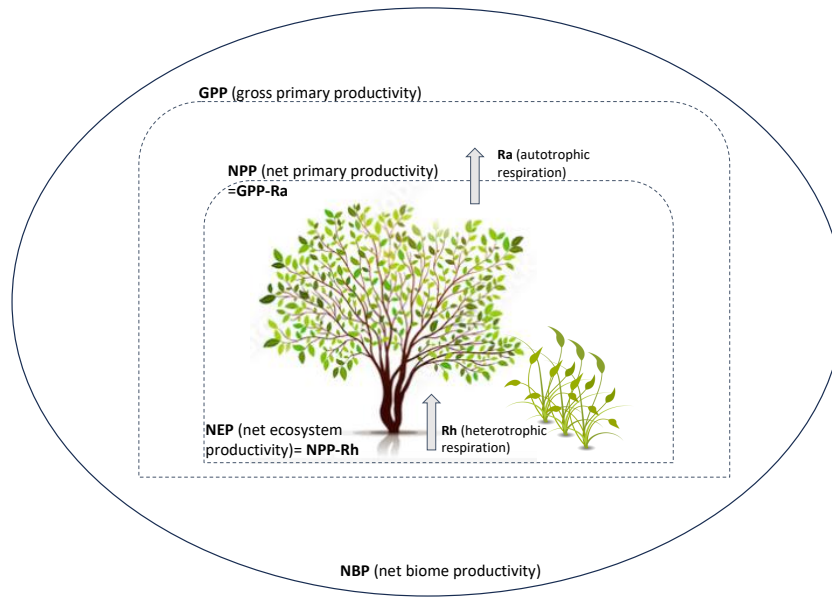



Figure 1. Distinction and interplay between GPP, NPP, NEP and NBP, with autotrophic (plants) and heterotrophic respiration. Inspired by Mancini et al. (2016).

1.2 Measuring productivity with optical Earth observation data

The presence of strong absorption features in optical wavelengths, which relate to biochemical properties such as pigment and water content, has led to a large body of research using optical sensors to monitor vegetation productivity, mitigating the need for direct measurements (e.g., Boisvenue et al., 2016; Brinkmann et al., 2011; Cai et al., 2021; Dusseux et al., 2022; Erasmi et al., 2021; Hill and Donald, 2003). Given the employment of optical sensors routinely recording data at different scales, generated data streams have gradually become a well-established source of information in a wide array of vegetation monitoring applications, such as assessing climate change impact and carbon modelling (e.g., Campbell et al., 2022; Wocher et al., 2022), drought monitoring (e.g., Atzberger et al., 2013) or biodiversity assessment (e.g., Lausch et al., 2020).

Traditionally, spectral vegetation indices (VIs) have been used to derive plant productivity metrics (e.g., Erasmi et al., 2021; Fiore et al., 2020). Advanced studies focused on dynamically integrating vegetation traits within more complex data-driven and process-based models to estimate GPP (e.g., Ardö, 2015; Pei et al., 2022). For instance, light use efficiency (LUE) schemes (Monteith, 1972) can model GPP as a function of the amount of incoming photosynthetically active radiation (PAR) and the fraction of absorbed PAR (fAPAR) along with an LUE term (e.g., Zhao et al., 2005; Wang et al., 2017). See also the extensive review by Pei et al. (2022) and seminal papers by Moulin et al. (1998) and Delécolle et al. (1992). VIs that are sensitive to fAPAR and related vegetation traits (e.g. chlorophyll

content, leaf area index: LAI) have been integrated into LUE-based approaches to represent physiological constraints on GPP (e.g., Gitelson et al., 2003; Cheng et al., 2014b; Xie et al., 2019). Data-driven RS-based approaches may include the establishment of statistical relationships through empirical approaches or, more recently, with machine learning (ML) algorithms (see review by Liao et al. 2023). Over the last decade, solar-induced fluorescence (SIF) from space measurements has become increasingly popular, giving a more direct measure of photosynthetic activity and thus serving as perhaps the most straightforward remotely sensed proxy for GPP (e.g., Frankenberg et al., 2011; Guanter et al., 2012).

In the most complex modeling approaches, GPP is inferred using process-based dynamic vegetation models (DVM) (e.g., Krinner et al., 2005; Sitch et al., 2003; Liu et al., 2014). DVMs can be both diagnostic and prognostic tools, able to simulate responses to climatic change including prognoses of carbon budgets (e.g., Rayner et al., 2005; Ardö, 2015). Ardö (2015) suggested that the integration of the realistic processes simulated by DVMs with high-resolution RS observations (i.e., in the form of VIs, and traits) may support more accurate productivity metrics estimation. These approaches are discussed in more detail in Sect. 3.

Overall, the development of methodologies is further accelerated by a vast increase in the long-term vision of EO data, the availability of historical data, and enhanced facilities through numerous data repositories. Subsequently, data analytics and data-driven ML methods have helped the spread and penetration of these (big) data into data-based services worldwide (Liu, 2015; Gorelick et al., 2017).

2   Sensor platforms for vegetation productivity monitoring

Over the last two decades, the optical EO domain has seen an increasing number of space missions with various sensors aboard, complemented by airborne campaigns and *in situ* measurements from widespread ground-based networks. This increase in the abundance of EO data has contributed to the establishment of consistent global databases with quality-checked optical data, which can be used to estimate vegetation productivity metrics, such as GPP, NPP, AGB, yield, among others (see also blue box) at almost any spatial and temporal scales (Kuenzer et al., 2015). The relevant sensor platforms serving to collect observations for deriving vegetation productivity information are graphically illustrated in Fig. 2 and described in the following sections.

2.1   Time series from EO satellites

In recent years, the availability of free satellite data has dramatically increased, amounting to petabytes of data. This expansion is due to the decreasing costs of data acquisition and the constant reduction of required computational resources and storage infrastructure. The review by Ustin and Middleton (2021) provides a detailed description of this trend. The availability of such data reinforces the usefulness of satellite data streams for capturing vegetation dynamics at various spatial scales, from monitoring local ecological habitats to conducting global studies (Cavender-

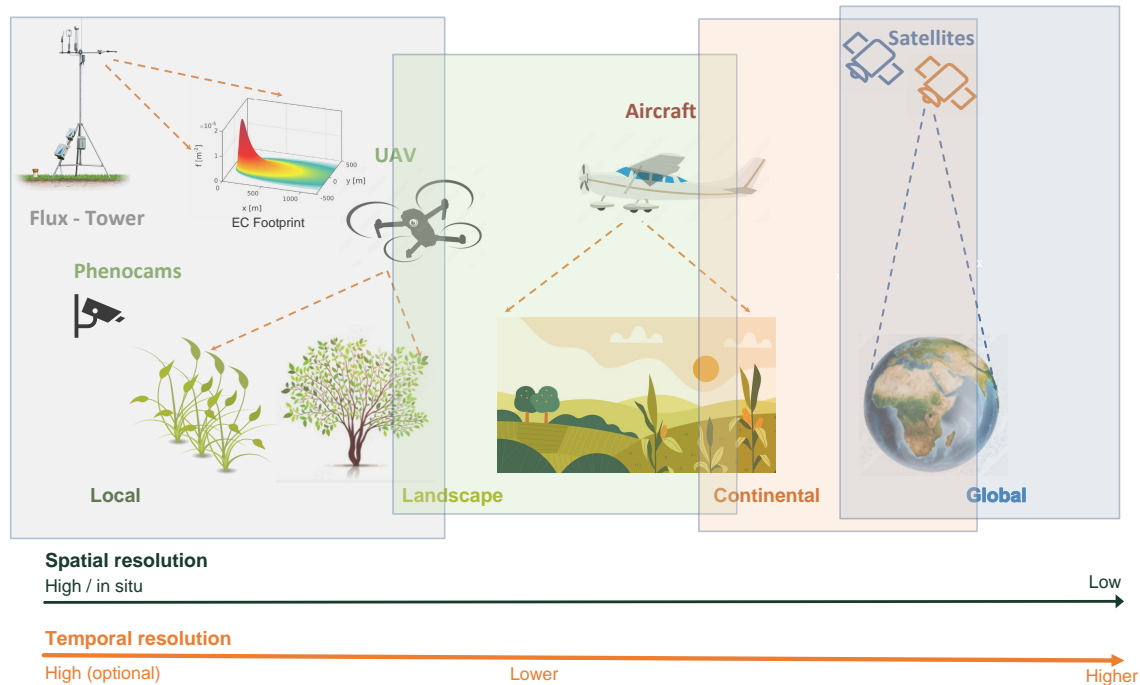



Figure 2. Overview of near and RS platforms used for vegetation productivity related TS analysis, i.e., flux towers with an exemplary footprint, phenocams, UAVs, aircraft, and satellites. The platforms are arranged in order from left to right, starting with the highest spatial resolution and progressively decreasing (i.e., from high to low), although EC footprint sizes may vary. In terms of temporal resolution, the leftmost platforms, i.e., phenocams, typically offer higher optional temporal resolutions. Moving towards the right, the temporal resolution decreases (e.g., with aircraft platforms), and then it increases again as we transition towards EO satellite platforms. Figure elements are own creations, except for the flux tower and EC footprint (Kljun et al., 2015).

Bares et al., 2020). Fig. 3 summarizes the available optical (main) sensors starting from the 1970s with their spatial resolution and revisit time.

Low Elevation Orbit (LEO) satellites have aboard sensors scanning at moderate (i.e., hecto- to kilo-metric) spatial resolutions, such as the Advanced Very High-Resolution Radiometer (AVHRR), Moderate Resolution Imaging Spectroradiometer (MODIS), Visible Infrared Imaging Radiometer Suite (VIIRS), PROBA-V (Project for On-Board Autonomy - Vegetation), and Ocean and Land Colour Instrument (OLCI) onboard Sentinel-3. They provide high frequency and long-term TS and thus support a deep investigation of the land surface phenology and trends along with a thorough monitoring of vegetation productivity of the entire Earth (see reviews by Zeng et al. (2020); Pipia et al. (2022a)). On the other hand, Geostationary Earth Observation (GEO) satellites offer an opportunity to capture rapid changes in vegetation dynamics thanks to their high revisit frequency, spanning over a few minutes. For

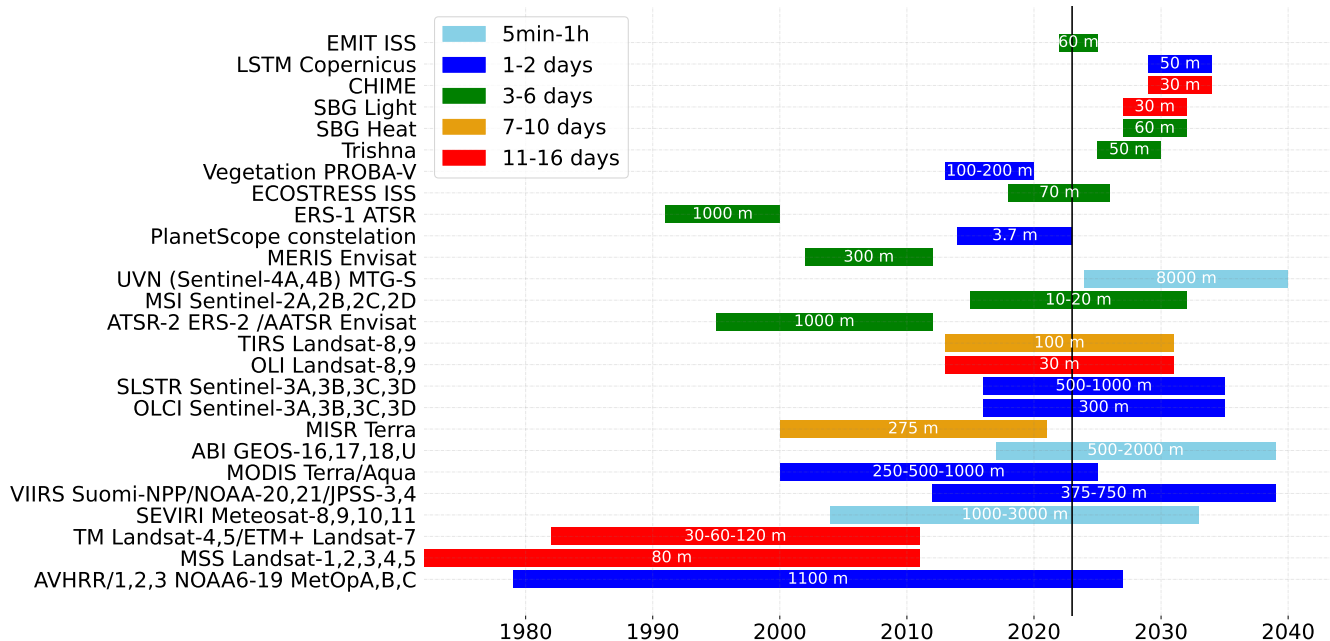



Figure 3. Optical EO sensors providing TS data starting from the 1970s. Different colours indicate the revisit time, and the spatial resolution for each sensor is given within the corresponding bars.

instance, mapping vegetation on an hourly basis by means of GEO satellites was explored by Fensholt et al. (2006), using the SEVIRI instrument onboard Meteosat Second Generation (MSG). Another mission of interest is NASA's Earth Polychromatic Imaging Camera (EPIC) onboard NOAA's Deep Space Climate Observatory (DSCOVR) (Yang
170   et al., 2017). The EPIC team's primary responsibility is to develop and validate algorithms that produce a series of products, including the vegetation green LAI (GLAI) and its sunlit portion, at a spatial resolution of 10 km. GLAI and its sunlit portion are critical state parameters in many ecosystem productivity models (e.g., Bonan et al., 2003; Bi et al., 2022).

Launched in 2018, the ECOSTRESS mission onboard the International Space Station (ISS) delivers nominally
175   daily land surface temperature (LST) products in taking advantage of the fast orbiting ISS (note that the real revisit period for a given location is variable and depends on the instrument's orbital cycle on bord the ISS). The spatial resolution of the products is 70 m except for two products of 30 m, due to the low altitude (Li et al., 2021b). In addition to the opening of the Landsat archives in 2008, further momentum was gained through the European Sentinel missions (Berger et al., 2012). From 2015 onward, Sentinel-2 (S2) optical imagery has been offering unprecedented
180   perspectives on the temporal variability of plant productivity of different ecosystems, e.g. grasslands (Dusseux et al., 2022) or forests (Lin et al., 2019) and its divergence over fine spatial scales. Compared to earlier land satellite missions, such as MODIS or Landsat, S2 provides improvements in revisit time (5 days at the equator), spatial

resolution (10-20 m) and spectral configuration (more and narrower vegetation-related bands) (Drusch et al., 2012). A 5-day revisit time may still pose limitations in acquiring a satisfactory number of cloud-free scenes required to construct a comprehensive composite product for productivity modelling in a dynamic ecosystem. This constraint becomes particularly crucial during transitional phases such as bud-burst and senescence, as well as (a)biotic stress events or following rainfall in water-limited ecosystems like drylands. It is worth mentioning that the near-polar orbit of S2 allows for a higher number of acquisitions when approaching the poles. For instance, over the high arctic archipelago Svalbard, S2 images can be obtained twice a day, allowing for regional-scale mapping of plant productivity via LSP metrics (Karlsen et al., 2021). For continental Europe, continuous phenological mapping using S2 is today operational in the Copernicus pan-European High-Resolution Vegetation Phenology and Productivity product suite (HR-VPP) project (Tian et al., 2021). The exploitation of Sentinel-3 OLCI data even ensures a daily global coverage although at a moderate spatial resolution (300 m), but with a higher number of bands, allowing the derivation of essential vegetation traits for productivity monitoring studies (e.g., Yang et al., 2021b; Reyes-Muñoz et al., 2022).

Until recently, a fine temporal revisit time was at the expense of fine spatial resolution. However, a new generation of satellite constellations is breaking these formerly restrictive inter-dependencies (see Fig. 3) with, for instance, the PlanetScope satellites that offer multispectral images at 3 m spatial resolution in daily revisit intervals (Roy et al., 2021).

2.2   Time series from piloted aircraft and unoccupied aerial vehicles

Aircraft constitute flexible and adaptable platforms to explore new protocols of measurements, support applied studies (e.g., Cheng et al., 2014a; Atzberger et al., 2015), and therefore provide data for the derivation of productivity metrics. However, in contrast to orbital platforms, the regular acquisition of TS using an aircraft is a logistical and financial burden. This may explain why we could identify only a few studies that employed piloted aircraft to acquire optical TS for the estimation of vegetation productivity metrics, such as Damm et al. (2015) focusing on SIF. In this study, the authors conducted a thorough evaluation of the correlation between far-red SIF measured at 760 nm and GPP across three ecosystems, namely perennial grassland, cropland, and mixed temperate forest, using multi-temporal Airborne Prism EXperiment (APEX) acquisitions. The authors concluded that RS of SIF more consistently correlated to GPP than conventional greenness-based indices.

To capture time trends on a smaller patch scale, Unoccupied Aerial Vehicles (UAV) have emerged as a more efficient and cheaper option than aircraft. Theoretically, UAVs meet most requirements for TS acquisitions regarding covering high spatial, spectral, and temporal resolutions (Berni et al., 2009; Aasen et al., 2018). UAVs are flexible and in contrast to satellite systems may be deployed whenever weather conditions are favourable for a desired measurement. Also, UAVs offer the necessary flexibility to sample diurnal cycles, which are relevant to capturing trends in productivity. To date, a range of multi-spectral and a few science-grade hyperspectral sensors have become available on the commercial market (Aasen et al., 2018), allowing for even faster system integration. In terms of TS

analysis for productivity, so far UAV measurements have been mainly employed to fill gaps in satellite observations caused by cloudiness or sparse data (Dash et al., 2018; Alvarez-Vanhard et al., 2021). A recent phenotyping UAV study, however, collected UAV data from a soybean field trial at unprecedented temporal resolution (Borra-Serrano et al., 2020) which allowed fitting growth curves with high accuracy (>90%) to derive relevant traits but also seed yield.

2.3 Multi-sensor and multi-scale synergies for time series

As data from different platforms and sensor modalities provide complementary information in terms of spatial, spectral, and temporal domains, the fusion of RS observations is increasingly coming into focus. For example, in the review study by Berger et al. (2022), the synergistic usage of multiple optical spectral domains was described to detect the stress of crops. Since productivity is affected by crop stress, improved stress detection and monitoring would also help in productivity studies. While biotic and abiotic stressors can only be disentangled through synergistic multi-sensor usage, in productivity studies, this synergy may be less relevant. Instead, multi-scale approaches, for instance, by combining spectral information from aircraft, UAVs, and EO satellites (as described above) are more essential. In this way, advantages of at least two platform types can be explored, such as more frequent availability or higher spatial resolution data (e.g., Gevaert et al., 2015; Sagan et al., 2019; Alvarez-Vanhard et al., 2021). By providing a higher number of observations, multi-sensor fusion improves the spatiotemporal continuity through gap-filling, leading to higher consistency and accuracy of current satellite products related to vegetation productivity (e.g., Claverie et al., 2018; Manivasagam et al., 2019; Sadeh et al., 2021). Although not explicitly treated in this review, additionally, the fusion of synthetic aperture radar (SAR) and optical TS data can be beneficial for productivity monitoring in regions with frequent cloud coverage (e.g., Pipia et al., 2019; Mercier et al., 2020; Caballero et al., 2023).

3 Time series processing methods for vegetation productivity monitoring

This section introduces several methods for deriving productivity metrics from remotely sensed TS data, including trend analysis, land surface phenology, and process models. Each method has its own strengths and weaknesses, and the best approach to use will depend on the specific application. The final sub-chapter of this chapter will introduce a variety of toolboxes that can be used to process and analyze remotely sensed TS data and derive productivity metrics. By providing a comprehensive overview of the different methods and tools available, this chapter aims to help researchers and practitioners select the best approach to deriving productivity metrics from remotely sensed TS data for their specific needs.

3.1 Time series sources and pre-processing

3.1.1 Vegetation Indices

Spectral VIs are widely applied methods for monitoring trends and deriving plant productivity metrics (e.g., Gutman, 1999; Huete et al., 2002; Atzberger and Eilers, 2011a; Rasmussen et al., 2014; Kang et al., 2018; Zeng et al., 2020; Shammi and Meng, 2021). Certainly, the most widely used VI in EO observation TS analysis is the normalized difference vegetation index (NDVI) (Rouse et al., 1974; Tucker, 1979). Its popularity comes from the fact that NDVI explores the contrasting behaviour of reflectance in the visible red and near-infrared (NIR) spectral domains, which strongly relate to vegetation biomass and, by extension, canopy-level plant photosynthetic activity. NDVI has the great benefit of being available to the research community through long observational records of more than five decades, specifically from AVHRR, the Landsat series, and MODIS (e.g., Huang et al., 2021; Li et al., 2021a). In addition to NDVI, other VIs have also been used to model temporal variations in productivity, including the enhanced vegetation index (EVI), which also accounts for canopy background and atmospheric influences (Huete et al., 2002). Multiple studies have explored TS of NDVI and EVI with direct linkages to vegetation productivity metrics, such as GPP (e.g., Shi et al., 2017; Shammi and Meng, 2021), or as part of GPP assimilation schemes (e.g., Zhang et al., 2015; Liu et al., 2021a). However, biomass-sensitive VIs often overestimate GPP at the start and end of the growing season, when leaf chlorophyll content decouples from LAI (Croft et al., 2014, 2015). Recently, novel VIs have been proposed for TS analysis, such as the Plant Phenology Index (PPI, Jin and Eklundh 2014), which is used for the calculation of the HR-VPP product at 10 m resolution as part of the Copernicus Land Monitoring Service (Tian et al., 2021).

Despite their widespread usage, spectral VIs also suffer from several drawbacks. Reducing the spectral signals into simple indices intrinsically leads to remaining spectral information unexploited, which potentially could inform about plant physiology (e.g., Atzberger et al., 2011; Verrelst et al., 2019a). In general, these parametric methods neglect the effect of the background soil and other confounding factors (e.g., Darvishzadeh et al., 2008; Verrelst et al., 2008, 2010; Gao et al., 2022). Also, they tend to be proxies for a small set of the physiological properties of vegetation only, leaving their empirical biophysical and biochemical meaning often ambiguous (e.g., Myneni et al., 1995; Morcillo-Pallarés et al., 2019).

3.1.2 Quantitative traits

A more explicit cause-effect alternative to obtaining TS of VIs can be derived from the radiative transfer theory. Radiative transfer models (RTMs) offer the possibility of deriving biochemical and biophysical traits at leaf (e.g., Jacquemoud et al., 1996; Ceccato et al., 2001; Féret et al., 2017) and canopy levels (e.g., Myneni et al., 1997; Rautiainen, 2005; Richter et al., 2009; Darvishzadeh et al., 2011) from optical remotely sensed data. RTMs describe the relationship between biochemical and biophysical traits and plant optical properties based on physical laws. Various inversion strategies have been developed based on lookup tables, numerical optimization methods and ML

methods, i.e. so-called hybrid approaches. An overview of RTM-based retrieval methods is provided by the reviews of Kimes et al. (1998); Baret and Buis (2008); Verrelst et al. (2015a, 2019a). Building upon these RTM inversion strategies, a few traits are operationally retrieved from routinely acquired EO data of land missions such as MODIS or S2. The most widely produced vegetation products are LAI and fAPAR, but also fractional vegetation cover, and to a lesser extent canopy chlorophyll content (e.g., Myneni et al., 2015; Yan et al., 2016; Fang et al., 2019; Xu et al., 2022). To obtain productivity metrics, TS data streams of the traits have been integrated into various GPP assimilation schemes (e.g., Jung et al., 2007; Xie et al., 2019; Chen et al., 2022).

Apart from those routinely generated vegetation products, a wide range of experimental studies present alternative retrieval methods or focused on the retrieval of other biochemical traits, e.g. leaf and canopy water content, leaf chlorophyll content (e.g., Croft et al., 2020; Estevez et al., 2021; Caballero et al., 2023). Typically, these studies have been limited to the processing of single-date observations or at best multi-temporal acquisitions for a restricted time window. Given those experimental retrievals, efforts to provide TS of a range of biochemical and biophysical traits were conducted by a few studies (e.g., Verger et al., 2016; Salinero-Delgado and Verrelst, 2021). An important note on the use of RTMs to derive quantitative traits concerns their sensitivity to phenological developmental stages of vegetation: Schiefer et al. (2021) demonstrated that trait retrieval accuracy has a strong dependency on phenology. A possible solution would be to use expert knowledge and *in situ* data to enable a more precise parameterisation of the RTMs depending on the phenological (macro) phase. At the same time, fast processing speeds are required to retrieve traits from TS data streams. This points towards hybrid retrieval schemes including active learning, i.e., relying on tuning RTM simulations against *in situ* measured traits and training of ML algorithms (e.g., Verrelst et al., 2021; Berger et al., 2021).

An overview of widely used quantitative traits in TS processing available from RTM inversion, and their potential relationship to vegetation productivity is given in Table 1. These traits can be further used within defined methodologies to derive productivity metrics given in the blue box, such as GPP. The capability of advanced RTMs such as SCOPE (Soil Canopy Observation, Photochemistry and Energy fluxes, Van der Tol et al. (2009); Yang et al. (2021a)) to model SIF is promising. SIF is a strong proxy for actual photosynthetic activity in canopies (e.g., Porcar-Castell et al., 2014; Verrelst et al., 2015b, 2016), and over the years various SCOPE-based SIF retrieval schemes have been proposed to derive GPP, usually by taking ecosystem-specific characteristics into account (e.g., Damm et al., 2015; Norton et al., 2019; Pacheco-Labrador et al., 2019; Yang et al., 2022).

3.1.3 Gap-filling and smoothing methods

Continuous, complete, and unbiased TS data is often a key requisite to monitor vegetation productivity using optical EO sensors. Here, one of the biggest challenges is data gaps. In reality, the availability of continuous data is often hampered by: (1) sub-optimum to inadequate weather conditions, such as clouds, snow, dust and aerosols (e.g., Kandasamy et al., 2013) or (2) instrumentation errors and uncertainties (Graf et al., 2023), as well as calibration issues (e.g., Brinckmann et al., 2013). Cloud cover is the most stringent limitation of optical satellite data. The

Table 1. Overview of widely-used biophysical variables inferable from RTM inversion to assess vegetation productivity information.

Trait	Description	Key references
Green leaf area index (GLAI)	GLAI quantifies the photosynthetically active foliage area and is proportional to gross photosynthesis and an important driver of net primary production.	Myneni et al. (2002); Baret et al. (2007, 2013)
Fraction of absorbed photosynthetically active radiation (fAPAR)	FAPAR refers to the amount of incoming solar radiation absorbed by live vegetation in the spectral range from 400–700 nm, divided by the total amount of absorbed radiation.	Knyazikhin et al. (1998); Myneni et al. (1997); Gobron et al. (2006)
Leaf chlorophyll content (LCC)	LCC refers to the total chlorophyll a+b content per unit leaf area (μg/cm^2). Chlorophyll molecules are responsible for harvesting the incoming PAR required to drive the light-dependent reactions of photosynthesis. LCC is closely related to leaf photosynthetic capacity.	Croft et al. (2020, 2017); Luo et al. (2019)
Canopy chlorophyll content (CCC)	CCC as the product of (G)LAI and LCC quantifies the amount of photosynthetically active radiation absorbed by a canopy and therefore relates to primary productivity.	Ali et al. (2020); Gitelson et al. (2014, 2015)
Solar-induced fluorescence (SIF)	SIF is an electromagnetic signal emitted by chlorophyll a of photosynthesizing plants and provides a mechanistic proxy for photosynthesis.	Frankenberg et al. (2011); Guanter et al. (2012); Porcar-Castell et al. (2014)

majority of the terrestrial Earth's surface is more or less regularly covered by clouds, and for some areas, persistent cloud cover can last for weeks (e.g., Atkinson et al., 2012; Wilson and Jetz, 2016). In such cases, data sparsity leads to biased estimates, decreased statistical power, increased standard errors, and substantial uncertainty in findings (Dong and Peng, 2013). For instance, clouds can mask key stages of phenological events, leading to unreliable monitoring practices such as productivity predictions (e.g., Karlsen et al., 2018). Notably, the amount of data gaps and noise strongly depends on the season, topography, location or environment (e.g., Beck et al., 2006; Vuolo et al., 2017).

The spatiotemporal gap-filling of missing TS data has therefore become a crucial step for monitoring the life cycle of vegetation and inter- and intra-annual variations in plant productivity (e.g., Beck et al., 2006; Schwartz, 2013; Kovács et al., 2023; Belda et al., 2020a; Amin et al., 2022). A high-quality signal can be assumed to represent the true seasonal trajectory of vegetation and should be carefully processed to retain the short-term character of data (e.g., using smoothing filters or splines). Signals with a high degree of noise need to be constrained by fitting to a predefined function to avoid unrealistic variations (e.g. asymmetric Gaussian or logistic functions). TS filters and splines can to some degree balance between retaining or smoothing short-term variations, and with these methods, parameter settings can be defined that balance smoothness with fidelity to the data (Atzberger and Eilers, 2011b). Important considerations when applying smoothing to TS data are whether data should be fitted to the upper envelope to compensate for signal bias (Chen et al., 2004; Jönsson and Eklundh, 2004), how to treat data points labelled as sub-optimal quality (e.g. cloud shadow pixels), and how to handle long periods of missing data (Beck et al., 2007; Jönsson et al., 2018; Bolton et al., 2020). Gap-filling and smoothing methods can be categorized into (1) smoothing and interpolation methods, (2) data transformation methods, and (3) fitting methods (Kovács et al., 2023). An exhaustive overview of available methods is provided in recent reviews by Zeng et al. (2020) and Pipia et al. (2022b), and is therefore not repeated here.

3.2 Assessment of vegetation productivity using trend analysis and anomaly detection

Long TS data streams of VIs (Sect. 3.1.1) or quantitative traits (Sect. 3.1.2) are particularly well suited for trend analysis, a widely used method for monitoring plant productivity (Eastman et al., 2009). Such analysis includes aspects such as abrupt or gradual changes in trends, as well as timing, number, and direction of such changes (Verbesselt et al., 2010). An example of TS decomposition is shown in Fig. 4. Each of these components can be further analyzed, for example, using separate trend models for annually derived attributes (Stellmes et al., 2013; Munawar and Udelhoven, 2020).

Regarding trend analysis, the study by Karkauskaite et al. (2017), for instance, explored data from MODIS (from 2000 to 2014) to evaluate the performance of PPI, NDVI and EVI in analyzing the trends of SOS in boreal regions of the Northern Hemisphere. The authors compared the VI trend results with *in situ* GPP-retrieved SOS from a network of flux tower observations. Although all three VIs produced similar trends in SOS, a pronounced land-cover

dependence was observed, with PPI-SOS outperforming the other two spectral indices in approximating vegetation productivity, i.e. GPP.

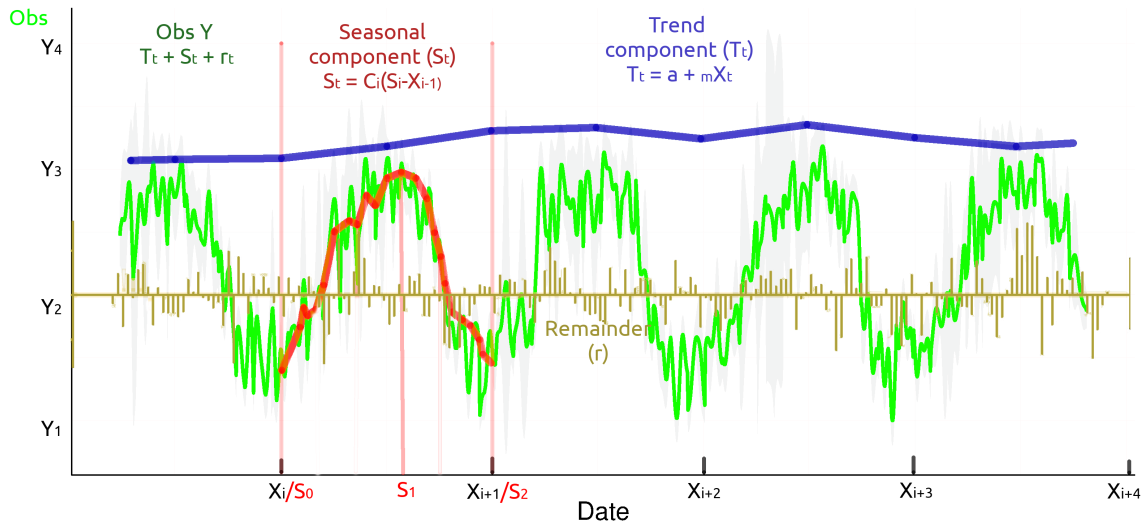



Figure 4. Generic plot showing the different components for TS analysis. Point observations result from the coupling of a general trend, a seasonal component, and a remainder quantity. The decomposition allows for measuring the trend at specific points, by disentangling seasonal effects.

In the context of anomaly detection, specific indices have been proposed: the Vegetation Condition Index (VCI) (Kogan, 1995) informs about overall vegetation conditions by referencing actual NDVI values with long-term statistics over the same period. The main application of VCI is related to drought detection (Klisch and Atzberger, 2016; Rembold et al., 2015a). Similarly, the Vegetation Productivity Index (VPI) (Smets et al., 2015) was proposed to detect anomalies in vegetation productivity. Importantly, these methods were developed for natural ecosystems such as boreal forests or sub-tropical savannahs where the vegetation type is assumed not to change from year to year. Thus, these indices are not appropriate for ecosystems with regular changes in species composition; e.g., agricultural croplands with crop rotation schedules. A deep learning approach for forecasting VCI was presented by Lees et al. (2022), demonstrating the usefulness of detecting drought conditions in Kenya using this anomaly index.

In addition to decomposing and analyzing trend patterns of a VI TS, an option is linking the VI to other environmental variables that influence vegetation productivity using distributed lag models (Udelhoven, 2011). However, relationships between climatic variables and responses in VI TS tend to be non-linear, spatially non-stationary and

sensitive to the scale of analysis. Simple regression model techniques such as Ordinary Least Squares (OLS) fail to model vegetation productivity accurately. To overcome such shortcomings, geographically weighted regression (GWR) approaches were suggested (Georganos et al., 2017).

3.3 Assessment of vegetation productivity using land surface phenology

Land surface phenology describes the seasonal timing and duration of vegetative growth using TS of VIs (Sect. 3.1.1) or biophysical variables (Sect. 3.1.2) (De Beurs and Henebry, 2004). Typical LSP metrics are dates and values for the start of the season (SoS), end of the season (EoS), length of the growing season (LoS), the peak of the season (PoS), season amplitude, and steepness of the greening and browning periods (Reed et al., 1994; Beck et al., 2006). Depending on the vegetation type studied, varying names can be found in the literature, such as the onset of greenness and the start of senescence for deciduous forests (e.g., Duchemin and Courrier, 1999; Kang et al., 2003; Badeck et al., 2004). A diversity of mathematical methods have been proposed for extracting the metrics from smooth seasonal trajectories. Most are based on absolute or relative thresholds of the seasonal amplitude (e.g., Bolton et al., 2020; Jönsson and Eklundh, 2004), whereas others are purely mathematical parameters, such as inflexion points or derivatives of different order (e.g., Fisher et al., 2006; Elmore et al., 2012; Melaas et al., 2013). A comprehensive review of the definition and extraction of LSP metrics is provided by Zeng et al. (2020).

Commonly, LSP metrics are used to study the impact of environmental changes on ecosystems: shifts in LSP, e.g., the earlier timing of SoS, indicate climate change (Abbas et al., 2021). For instance, Wood et al. (2021) used three decades of AVHRR data over the U.S. Northwestern Plains to study the impact of climate change and agricultural management on phenology. They concluded that climate factors such as precipitation and temperature can have a significant impact on productivity, but other factors such as soil nutrients, disturbance, and management practices also play a role.

The concept of LSP also has its drawbacks. Apart from the influence of the smoothing technique and the method used to extract the LSP metrics, Helman (2018) stressed that changes in vegetation species composition rather than phenological transitions could produce a false-positive signal in LSP. Moreover, LSP metrics show high sensitivity to the frequency and temporal coverage of observations as well as cloud contamination, which can affect the estimation of productivity metrics (Younes et al., 2021).

3.4 Assessment of vegetation productivity using dynamic process models and data assimilation

A more advanced perspective is given by combining remotely sensed TS data with simulations of plant physiological processes and their temporal development. Simulated plant growth driven and/or constraint by TS data streams and environmental covariates can be used to study processes that are not directly quantifiable from the satellite data itself - such as the amount of AGB increase over time (Delécolle et al., 1992). Here, EO data offer the possibility of providing a dynamic, spatially continuous parameterisation of model input variables (e.g., Bach and Mauser, 2003; Verhoef and Bach, 2003; Hank et al., 2015).

Process-based dynamic vegetation models can have different levels of complexity concerning their ability to simulate biophysical and biochemical processes in plants (e.g., Quillet et al., 2010; Ardö, 2015). Based solely on empirical data, canopy structure dynamics models (CSDM) have been proposed to simulate a TS of canopy traits such as LAI as a function of temperature (growing-degree-days) (e.g., Baret et al., 2000; Koetz et al., 2005). Using the concept of LUE, Goudriaan and Monteith (1990) described vegetation dry matter accumulation as a function of leaf area expansion. By including further knowledge about physiological processes and plant morphology, more advanced DVMs can be created to simulate ecosystem productivity such as for boreal forests (e.g., Liu et al., 1997) or croplands (e.g., Delécolle et al., 1992; Launay and Guerif, 2005; Liu et al., 2016). For instance, The Breathing Earth System Simulator (BESS) model (Ryu et al., 2011; Jiang and Ryu, 2016) couples atmosphere and canopy processes, two-leaf photosynthesis, energy balance, to provide evapotranspiration and GPP.

Fischer et al. (1997) already distinguished three different strategies to combine remotely sensed TS of vegetation with process-based models, which can be seen as state-of-the-art, as delineated in Fig. 5: (1) model forcing, (2) model recalibration, and (3) coupled forward modelling. In the model forcing strategy (Fig. 5, 1), the remotely observed state variables (e.g., fAPAR, LAI) are forced (input) into the process model (e.g., BESS by Tagliabue et al., 2019). In the recalibration strategy (Fig. 5, 2), also known as 'data assimilation', remotely sensed state variables are used to readjust DVM parameters or inputs whenever an observation becomes available. While the first two strategies involve inverse modelling to obtain the remotely sensed state variables, the third approach relies entirely on forward modelling (Fig. 5, 3). It couples a DVM with an RTM to simulate vegetation optical properties, which are then compared to remotely sensed data. The main advantage of this strategy is the avoidance of inverse modelling, which is not only ill-posed but usually also computationally intensive. Shiklomanov et al. (2021), for instance, coupled three existing models, namely the Ecosystem Demography model version 2 (ED2, Medvigy et al., 2009), PROSPECT-5 (Feret et al., 2008) and a simple soil reflectance model to the EDR model. Their model predicts the full range of high-spectral-resolution surface reflectance, which is dependent on the current state of the ED2 model. Another relevant example is provided by Wang et al. (2023) with Climate Modeling Alliance (CliMA) Land, which is able to simulate data streams of productivity metrics such as GPP, transpiration, as well as canopy reflectance and fluorescence spectra that can be observed by satellites in a high temporal resolution. The authors demonstrated the potential of CliMA Land in tracking the spatial patterns of productivity metrics (GPP) compared to data-driven methods. Similarly, Poulter et al. (2023) recently coupled the LPJ-wsl global DVM and the canopy radiative transfer model PROSAIL. LPJ-PROSAIL can generate global, gridded TS of daily visible to shortwave infrared (VSWIR) spectra (400–2500 nm) taking into account temporal and spatial variability. Overall, these studies demonstrate that the model couplings (DVM and RTM) are valuable tools for monitoring the development of vegetation activity at the global scale, in strong relation to the carbon cycle and hydrology. With this, the method can provide the prerequisite of the Digital Twin concept allowing to model productivity with high fidelity for longer time periods, and eventually evaluate different future scenarios.

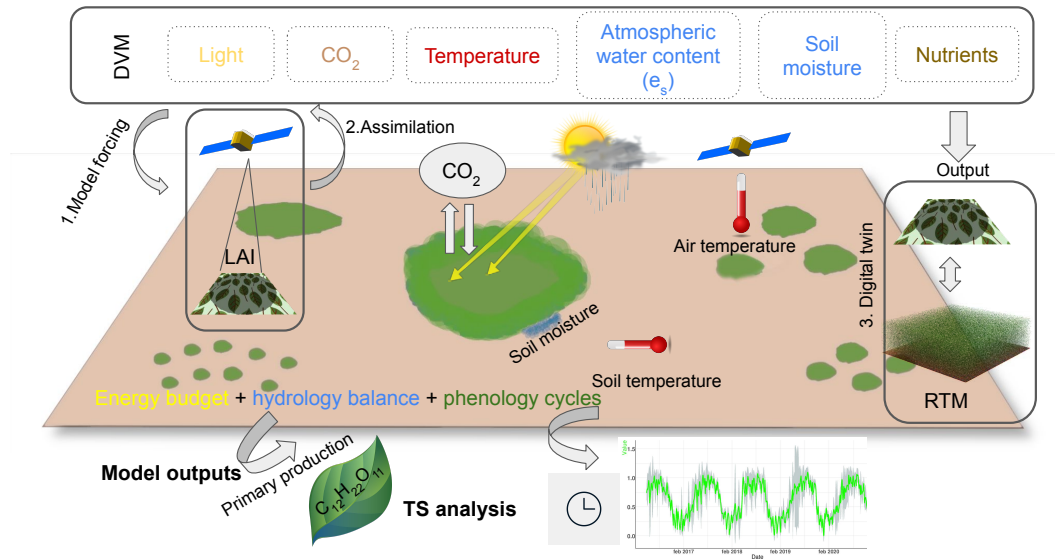



Figure 5. Three strategies to combine remotely sensed TS with process-based DVMs: (1) model forcing, (2) data assimilation (including model recalibration and re-initialization) and (3) coupled forward modelling of DVMs and RTMs (=Digital Twin).

3.5 Toolboxes for vegetation productivity studies

A variety of sophisticated software packages have been developed to facilitate the processing and analysis of large image TS and ultimately provide key information about vegetation dynamics and ultimately about productivity metrics. In most cases, these packages are openly available, and share common purposes, although they differ in specific features and methodologies. Broadly, we can distinguish toolboxes for TS processing, TS analysis and change detection, traits retrieval, and process modelling (i.e., DVM). Tab. 2 lists the toolboxes according to this categorization, including functionalities and implementation. Note that we have compiled this list to the best of our knowledge; however, it is possible that it may not include all existing toolboxes.

TIMESAT (Jönsson and Eklundh, 2004), for instance, is able to transform noisy signals into smooth seasonal curves and to extract seasonality metrics, like SoS, EoS, and LoS, or integrated values. Originally developed for coarse spatial resolution data (e.g. AVHRR or MODIS), with mostly equidistantly spaced temporal observations, recent versions have adopted the characteristics of satellites with high spatial resolution but infrequent temporal observations, such as Landsat and S2. While TIMESAT uses least-squares methods, the Decomposition and Analysis of Time Series software (DATimeS) (Belda et al., 2020a) expands established TS interpolation methods to over 20 conventional (e.g., Whittaker smoother (Eilers, 2003)) and advanced ML fitting algorithms, like Gaussian process regression (GPR), which is particularly efficient for reconstructing multi-seasonal vegetation patterns (Belda et al., 2020b). In this way, DATimeS provides interpolated VI/trait values from unevenly spaced TS and associated uncertainties and allows extraction of phenological metrics for each crop and season. DATimeS then also enables the calculation of

Table 2. Toolboxes recommended and used for converting remotely sensed TS into gap-filled VI and vegetation trait products, and to derive LSP metrics and trends, which all can be ultimately used for estimating productivity metrics. Note that this list is not necessarily exhaustive, but rather a selection of some of the most notable tools that we are aware of, to the best of our knowledge.

Toolbox (link)	Functionality	Implementation	Reference
TS processing:			
TIMESAT	Gap-filling / phenology metrics	Standalone	Jönsson and Eklundh (2004)
DATimes	Gap-filling / phenology metrics / TS fusion	Matlab GUI	Belda et al. (2020a)
TS analysis and change detection:			
TimeStats	Trend, seasonal, and multivariate analysis	IDL virtual machine	Udelhoven (2010)
EOTSA	Trend, seasonal, and multivariate analysis	Web interface, RStudio	Leopold et al. (2020)
BFAST	Phenology metrics / breakpoint analysis	R Studio	Verbesselt et al. (2010)
HiTEmpo	Model-based change detection algorithm	-	Van Den Bergh et al. (2012)
SPIRITS	Indicators / anomalies	Java virtual machine	Eerens et al. (2014)
R libraries	Indicators, analysis, visualisation	R	e.g., Araya et al. (2018)
Traits retrieval:			
EnMAP-Box 3	Data-agnostic handling of multi-sensor TS data	Python, QGIS plugin	van der Linden et al. (2015)
ARTMO	Quantitative traits / RTMs, ML	Matlab GUI	Verrelst et al. (2012)
Process modelling:			
PCSE	DVM forward modelling, satellite data assimilation	Python	-

445 the same seasonality metrics as TIMESAT, and also has built the option to fuse TS of two data sources, e.g. optical and radar data (Pipia et al., 2019). Apart from TIMESAT and DATimeS, there are other software tools to analyse VI TS data for phenology-related studies including Phenological Parameters Estimation Tool, enhanced TIMESAT, Phenosat, CropPhenology and QPhenoMetrics (Zeng et al., 2020).

TimeStats (Udelhoven, 2011) goes beyond the extraction of phenological metrics as it expands TS analysis methods 450 to parametric and non-parametric methods for trend detection, generalized-least square regression, distributed lag models, cross spectra analysis, windowed trend and frequency analysis, continuous wavelet transform, and empirical mode decomposition. Based on some of those methods within TimeStats, predefined workflows were implemented in a web interface called EOTSA (Earth Observation Time Series Analysis) Toolbox (Leopold et al., 2020). EOTSA allows online access to satellite data archives (currently the full PROBA-V database) without the need for local 455 data storage. Fig. 6 shows two examples where NDVI TS were analysed at the continental scale using EOTSA. In the first example, seasonal characteristics (mean NDVI, annual magnitude, peaking time) were derived (step 1), followed by a trend analysis (step 2) (Fig. 6B). The colour composite of the trends for the seasonal characteristics reveals spatiotemporal patterns. Fig. 6C shows an example of multivariate TS analysis in which NDVI was regressed against lagged rainfall using distributed lag modelling after pre-whitening the TS. Regions with positive correlation

460 at higher lags depict the dependence of vegetation biomass production on accumulated previous rainfall amounts. These can be for instance located in semi-arid areas occupied by natural grassland.

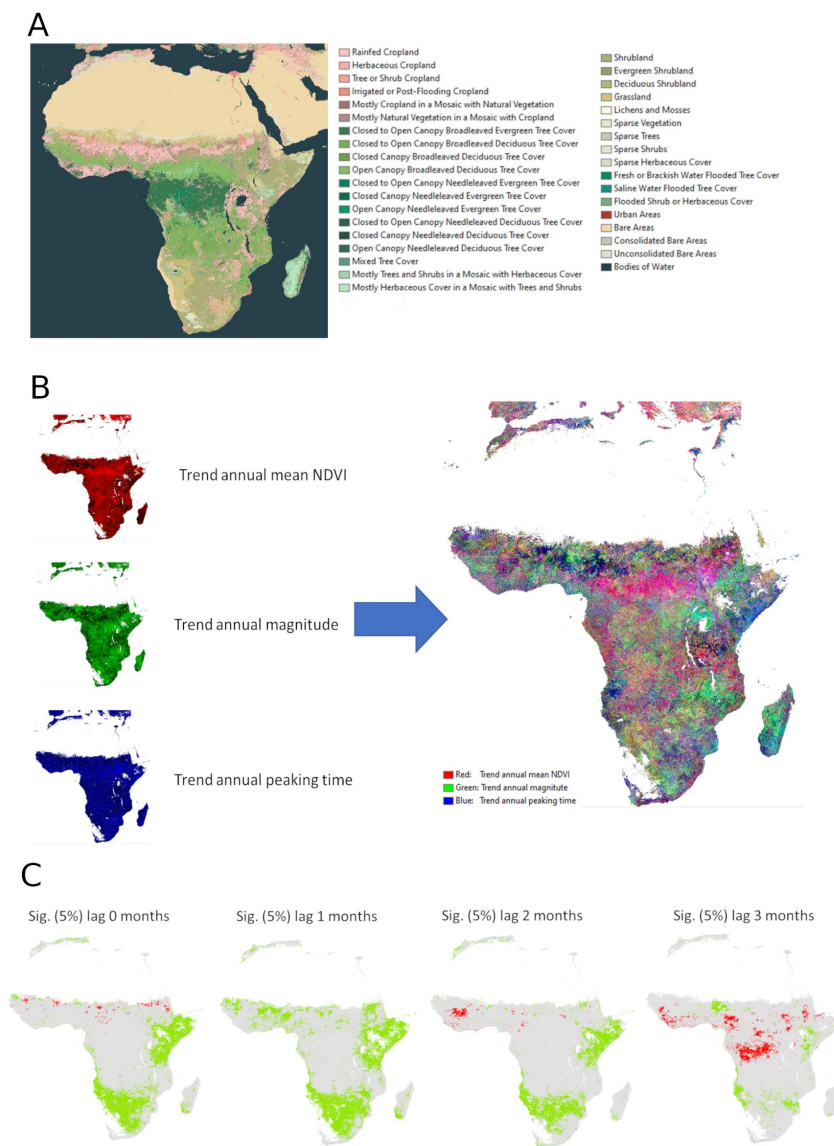



Figure 6. Landcover map of Africa and legend (A), trend analysis for a TS of MODIS satellite images (period: 2015-2019) displayed as RGB colour composite (B), results from Distributed Lag Modelling where NDVI was regressed against lagged rainfall (C). Prepared with EOTSA RStudio version.

BFAST (Verbesselt et al., 2010) is a generic change detection approach that considers seasonal, trend, and remainder components through iterative estimation of the time and number of abrupt changes within TS, and characterisation of change by its magnitude and direction typically applied in forest monitoring studies.

465   HiTempo (Van Den Bergh et al., 2012) is a software tool created to aid in the study of TS analysis of hyper-temporal sequences of satellite image data. The platform was specifically designed to simplify the exhaustive evaluation and comparison of algorithms while ensuring the reproducibility of experiments.

SPIRITS (Eerens et al., 2014) is a comprehensive software toolbox designed for environmental monitoring, with a particular emphasis on generating clear and evidence-based information for crop production and decision-makers.

470   SPIRITS provides a vast array of tools for extracting vegetation indicators from image TS and estimating the potential impact of anomalies on crop production (Rembold et al., 2015b). With its user-friendly graphical interface, SPIRITS offers an integrated and adaptable analysis environment that facilitates sequential tasking and provides a high degree of automation for processing chains.

The EnMAP-Box 3 (van der Linden et al., 2015) provides a user-friendly GUI with tools for collecting and

475   visualizing spectral profiles from various sources such as raster images. Furthermore, the QGIS processing framework has been expanded by incorporating many algorithms typically utilized in EO data and imaging spectroscopy analysis for a diversity of ecosystems. The "Agricultural Applications", for instance, provide empirical and physically based trait retrieval strategies which can be explored for deriving productivity information (e.g., Danner et al., 2021).

Regarding RTMs, the Automated Radiative Transfer Models Operator (ARTMO) toolbox (Verrelst et al., 2011)

480   is an outstanding example. ARTMO provides GUI-based access to several leaf and canopy RTMs, and atmospheric RTMs and offers sophisticated strategies for forward and inverse modelling including state-of-the-art ML methods.

Finally, there is a host of available R packages, e.g., CropPhenology, for extraction of crop phenology from TS based on VIs (Araya et al., 2018), the phenofit package - intended for daily vegetation TS and monitoring of vegetation phenology from satellite VIs (Kong et al., 2022), or LPDynR as a tool to calculate the Land Productivity Dynamics

485   indicator (Rotllan-Puig et al., 2021). Moreover, there are Python libraries for phenology and vegetation productivity apps available for ODC. The aim of the ODC initiative is to enhance the worth and influence of worldwide EO satellite data. It does so by offering an open and free-to-use data exploitation structure, and by encouraging a community to cultivate, maintain, and expand the technology and its range of applications (Killough, 2018).

While the aforementioned toolboxes focus on the usage of remotely sensed data only, we found only a few tools

490   that allow users to work with DVMs. Many DVMs are (often) based on FORTRAN programming and lack graphical user interfaces or high-level programming interfaces. The 'Python Crop Simulation Environment (PCSE) has ported old-style DVMs to modern Python programming but, still, considerable coding skills are required to make use of it. PCSE offers a platform for carrying out crop simulation modelling along with tools to read supporting data (such as weather, soil, and agricultural management) and components for simulating various biophysical processes

495   including phenology, respiration, and evapotranspiration. Additionally, PCSE features implementations of widely used crop and grassland simulation models like WOFOST, LINGRA, and LINTUL3. WOFOST, for instance, has

been employed in the operational crop yield forecasting system MARS, which is used to monitor crops and predict yields worldwide (De Wit et al., 2019; Lecerf et al., 2019). Furthermore, the code of specific process models has been made available via the specific websites of the model authors, e.g, the BESS model.

4 Validation of RS-based primary productivity estimates

Validation is a critical step in ensuring the accuracy and reliability of estimated quantities or (vegetation) products derived from remotely sensed TS data sets (Justice et al., 2000). The validation process involves comparing the estimates with those from independent sources, such as *in situ* observations, to evaluate their overall quality and suitability for a particular application. The comparison between remotely sensed data products and ground-based measurements enables the detection of errors and biases in the retrieved products and improves the interpretation and understanding of the underlying ecological processes (Wu et al., 2019). Ultimately, validation is essential for ensuring that remotely sensed TS data can be used to accurately estimate GPP, NPP, and other vegetation productivity metrics.

4.1 Validation strategies

In the context of productivity monitoring, we distinguish three distinct validation methods:

1. *In situ* validation;
2. Local sensor networks;
3. Multi-product intercomparison.

These methods are illustrated in Fig. 7, which showcases how they interplay to provide accuracy, time resolution, and spatial representation, as further elaborated below.

The first category, *in situ* validation (1.), involves comparing RS data products to direct ground-based observations of productivity metrics. Examples include the direct determination of AGB, litter biomass, and crop yield. In many cases, *in situ* data is collected by harvesting plots and determining dry biomass (e.g., Zhang and Zhang, 2016; Liu et al., 2021b). One prominent data set is the ORNL DAAC Net Primary Productivity data collection (ORNL DAAC, 2023). It comprises field measurements of AGB and estimated NPP from roughly 100 terrestrial study sites across the globe, including different types of forests, grasslands, and crops. These data were gathered from various published literature and other available sources of information. *In situ* validation provides a means of calibrating models to ensure consistency over time, which is essential for long-term studies.

The second category, sensor networks, (2.) is perhaps the most widespread and promising strategy for validating productivity products (i.e., metrics) from EO data. This category refers to a network of distinct sensors, comprising spectral radiometers, phenocams and eddy-covariance (EC) flux towers (e.g., Baldocchi et al., 2001; Baldocchi, 2003; Hilker et al., 2011; Toomey et al., 2015). Such an approach requires deploying validation sites or observation networks with standardized observation protocols (Morisette et al., 2006). The employment of spectroradiometers,

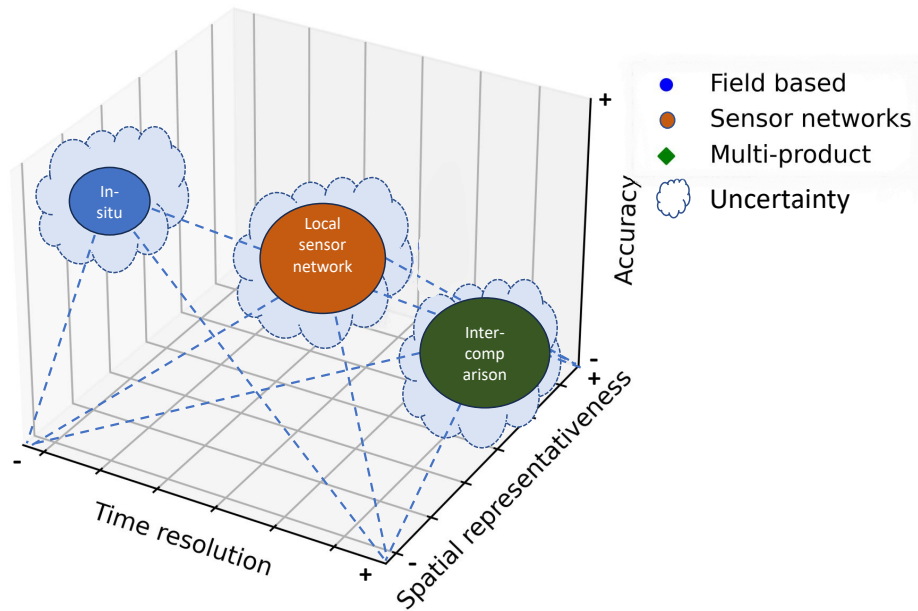



Figure 7. Interplay of the three main approaches (field-based: *in situ* validation, sensor networks and multi-products inter-comparison) of validating vegetation productivity, as a function of time, spatial representation and accuracy.

phenocams, and EC systems is a valuable tool for providing both continuous, high-resolution (i.e., sub-daily) esti-
mates of vegetation productivity over daily to decadal timeframes and also serving as validation for satellite-based
products. Phenocams capture time-lapse images of vegetation, allowing the monitoring of phenological events such
as leaf emergence, flowering, and senescence. This information is valuable for tracking the growth and development
of vegetation, as well as for identifying changes in productivity due to environmental stressors. For example, the
SpecNet network (SpecNet, 2022) aims to link optical measurements with flux sampling and standardized field op-
tical methods (e.g., Gamon et al., 2006, 2010). The Committee on Earth Observing Satellites (CEOS) Group on
Calibration and Validation is currently leading efforts concerning the development of best-practice phenology valida-
tion protocols and the establishment of ground-reference sites across different biomes (NASA, 2023). The use of EC
techniques for providing direct measurements of the exchange of carbon, water and energy between vegetation and
the atmosphere (Baldocchi et al., 2001) has provided an extremely valuable means of measuring plant productivity
across diurnal to decadal time scales. The longest-running flux tower is located in Harvard Forest and has been
providing continuous measurements at half-hourly intervals since 1989 (Urbanski et al., 2007). Several national and
regional networks of flux towers exist (e.g. Ameriflux, Chinaflux, Ozflux, ICOS), which has enabled the contribution

of EC data to improve our understanding of plant-environment interactions to go beyond a single site or ecosystem to regional-to-global studies. To address data consistency and allow cross-site comparisons, FLUXNET was established in 1997, which is a 'network of networks' and has led to harmonised methods and datasets. The latest dataset of FLUXNET, FLUXNET2015, contains gap-filled TS data streams of GPP, Re, and meteorological data for 1500 site years, along with an estimation of uncertainties (Pastorello et al., 2020). However, there are concerns about the spatial and temporal representative of EC data, due to the disproportionate predominance of flux towers being located in North America and Europe (Chu et al., 2017). To scale from the footprint of individual flux tower sites to gridded, spatially- and temporally-explicit products, a variety of ML techniques have been employed, including neural networks, regression trees and kernel methods (Beer et al., 2010; Jung et al., 2011, 2020). EO data is usually used, along with meteorological data within the ML algorithms, to extrapolate across time and space. These EC-derived products, such as those within the FLUXCOM initiative (Jung et al., 2020) have been extensively used in validating other sources of vegetation productivity estimates, including those from satellite-based EO data streams and terrestrial biosphere models (Chu et al., 2017).

The integration of these diverse ground-based sensing techniques together with EO data streams is suitable for monitoring large-scale vegetation dynamics, and it can aid in the interpretation and validation of productivity models obtained from remotely sensed data (Balzarolo et al., 2014). From a technical point of view, it is common to find literature that explores the accuracy of satellite imagery validated through such near-surface sensors. Additionally, there is increasing usage of similar networks focused on different aspects of vegetation and supported by the spread of low-cost and IoT sensors, for example, the TreeTalker network (Valentini et al., 2019; Tomelleri et al., 2022).

The third category, multi-product intercomparison, (3.) involves the benchmarking of multiple productivity products or different models using EO data. This validation approach requires a thorough comparison of the obtained products with similar ones to check for consistency (Beer et al., 2010; Lin et al., 2022; Meroni et al., 2012). A critical aspect of this approach is ensuring that the models or products being compared are fit for purpose. In other words, they must be appropriate for the specific application or use case. Additionally, the cross-comparison of distinct types of models, such as (an ensemble of different) DVMs and data-driven approaches (e.g., Ardö, 2015; Jung et al., 2020), can provide valuable insights into the strengths and weaknesses of each model type. Benchmarking models using EO data can help to improve their accuracy and reduce errors in their predictions, which is essential for applications such as monitoring global climate change and assessing the health of ecosystems. It can also aid in developing more advanced primary productivity models that can better account for the complexities of ecological processes and environmental variability.

4.2 Bridging the scaling gap

Scaling issues remain one of the most significant challenges in extracting vegetation productivity, regardless of the metric chosen (Zeng et al., 2020; Caparros-Santiago et al., 2021). The disparity in spatial and temporal resolution between *in situ* measurements and remotely sensed data often creates uncertainty in the extracted vegetation pro-

ductivity estimates. While *in situ* (point) observations are typically species-specific, RS platforms capture a mixture of vegetation types within their large geographic footprint. Consequently, directly comparing *in situ* and remotely derived productivity estimates can be difficult, if not impossible. Furthermore, while *in situ* observations or local sensor networks provide a high level of detail and accuracy, their geographical coverage is often limited and may not be indicative for large-scale studies (see also Fig. 7). In contrast, EO data products from multiple satellites offer broader coverage, but they suffer from coarser spatial resolutions. This trade-off between detail and coverage presents a significant challenge in scaling *in situ* observations or local sensor networks (categories 1) and 2) into the larger scale captured by EO data. Therefore, to overcome the scaling challenge and enhance the accuracy of remotely derived vegetation productivity metrics (see blue box in Sect. 1.1), an effective protocol for the calibration and validation of such metrics using *in situ* observations, sensor networks, and multi-product / model intercomparison is essential. See also the multiscale validation scheme as outlined in Malenovský et al. (2019).

5 Systematic literature review on time series based applications for vegetation productivity

This section aims to complement the previous sections by taking a tour across principal thematic applications through a meta-review. We do not assess the calculation of productivity applied in these studies. Instead, we aim to provide a thorough overview of how remotely sensed TS data were explored to estimate productivity for agricultural, forestry, and other natural ecosystem applications. In this way, readers will be redirected towards specific scientific studies analysing productivity with a multitude of proxies and methods for these application domains.

5.1 Systematic literature review

The systematic literature review followed the guidelines of the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) (Page et al., 2021). The SCOPUS and Web of Science web catalogues were queried for published, peer-reviewed studies. In SCOPUS, the title, abstract and keywords were searched with the query "time AND series AND productivity AND 'remote sensing' AND (vegetation OR forest OR crop)", while the topic field in the Web of Science catalogue was searched for "'time series' AND (vegetation OR forest OR crop) AND productivity". The resulting 915 records of the two databases were merged into one database by omitting duplicated records as identified by their DOI (Fig. A1). The records were further screened to include research articles and conference contributions in the English language, excluding review studies. Furthermore, the studies were required to use RS analysis of terrestrial vegetation with at least two observations in time. For each entry, a range of attributes was recorded (Tab. 3).

Unlike other studies, which defined a TS as consisting of a minimum of several observations, we included studies with a minimum of two images without an upper limit. This allowed us to include studies that have traditionally been labeled under the topic of change detection analysis. We chose to do this for two reasons. First, we believe that the minimum number of observations in a TS is arbitrary, and we wanted to take a more comprehensive approach

to examining the aspect of time. Second, the number of studies using long TS consisting of high-resolution (10-30
610   m pixel size) images is relatively small. Considering only long TS data streams would have excluded many studies
that observe productivity from Landsat and Sentinel-2 satellites.

Table 3. Attributes retrieved from selected studies for the systematic review.

Attributes	Definitions
Sensor/platform	Sensors and platforms used in the study
Spatial resolution	Ground sampling distance of primary data product used in the analysis (in metre)
Land cover	Land cover according to IGBP land cover classes[1], plus category of LULCC
Study area category	Size of study area in administrative terms (local, region, country, multi-country, continental, pan-continental, global)
Study area size	Size of study area (in km^2)
Time series start/end [date]	Start and end date of time series
Revisit	Frequency of observations in the time series (in days)
Time series steps	Number of observations between start and end date (alternative to revisit)
Definition productivity	Primary RS products used to derive productivity metrics (VI/LSP/traits/process/LULCC)

Fig. 8 shows the number of published papers per number of explored TS observations. Note that the x-axis starts
with "2". There is a skewed normal distribution with a median of 227 temporal observations and a long tail towards
a higher number of observations. The 75th percentile is reached at 786 observations.

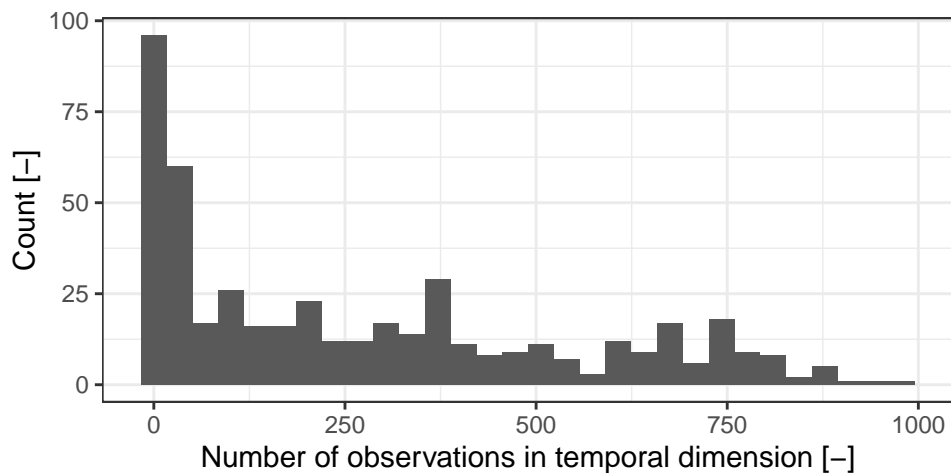



Figure 8. Histogram of number time steps used by the reviewed studies. Thirty-three studies with $\geq$1000 steps have been
removed in order to facilitate representation.

615   Fig. 9a summarises which RS-derived products or methods were used by the studies to approximate productivity. Note that some studies referred to productivity but did not specifically state if the generated products were meant to be a representation of productivity, this required care in the interpretation of the results. Generally, productivity proxies were categorized into (1) VIs, being the simple algebraic transformation of spectral observations (see also Sect. 3.1.1); (2) phenological metrics, i.e. derivatives of observations over time, as described in Sect. 3.3), (3) traits, i.e.

620 biophysical/ biochemical properties of vegetation at the time of observation (see also Sect. 3.1.2), (4) process, which implies the use of DVM (see also Sect. 3.4), and finally (5) land use and land cover change classifications (LULCC). VIs were most often employed to describe productivity, with almost 50% of all analyzed studies. Specifically, most studies relied on NDVI TS, which may be the most used and well-known method to analyse TS in the context of vegetation productivity. VIs were followed by traits, processes, and phenological metrics, and cover characteristics

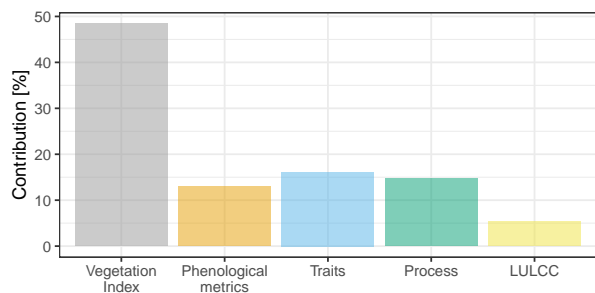
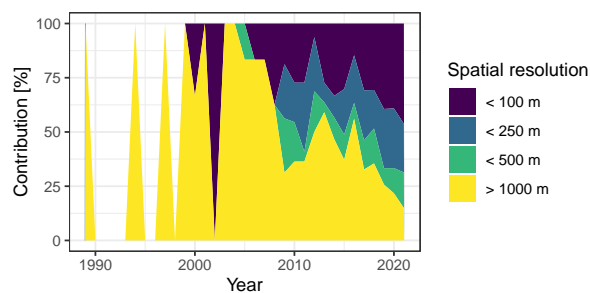
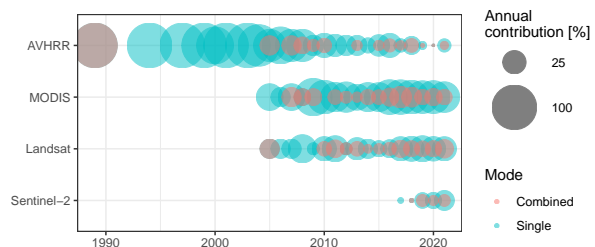
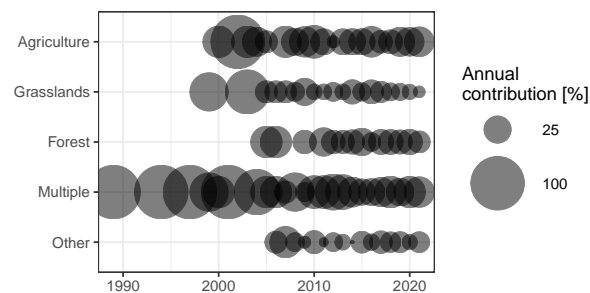
625 as less often used proxies.

(a) Definitions and RS products used in the context of vegetation productivity, i.e. to derive the productivity metrics, in reviewed studies.

(b) Trends in spatial resolutions (pixel size) at which spatial products were produced in reviewed studies.

(c) Trends in assessed aggregated land cover types in reviewed studies. The category "Other" includes studies covering multiple land cover types as well as land cover/land use change studies.

(d) Trends in assessed aggregated land cover types in reviewed studies. The category "Other" includes studies covering multiple land cover types as well as land cover/land use change studies.

Figure 9. Results of systematic literature review.

Fig. 9b and Fig. 9c show the trends in spatial resolution and sensors underlying the vegetation productivity studies, respectively. In both, three phases can be distinguished: first, the dominance of AVHRR-based and coarse-resolution studies until 2005 (e.g., Wessels et al., 2004). In this period, only 21 studies (3.7 %) were published. Second, a rising contribution of MODIS and Landsat marked the period from 2005 until 2017 (e.g., Boisvenue et al., 2016). During this period the number of studies per year increased from 6 (1.1 %) in 2005 to 52 (9.2 %) in 2017. In Fig. 9b, the years 2013 and 2016 appeared to be outliers with the highest portion of studies with larger than 1000 m resolution. The 2016 outlier can be explained with the publication of the Global Inventory Monitoring and Modeling System (GIMMS) third generation NDVI (NDVI3g) long-term TS dataset based on AVHRR (Pinzon and Tucker, 2014). The last phase started in 2017 and is marked by an increasing trend towards sub-1000 m resolution studies driven by the increased availability of longer-term Landsat and MODIS TS. Studies combining both sensors make up 6.3 % of all (e.g., Knauer et al., 2017; Kussul et al., 2017). Moreover, an unprecedented amount of other sensor TS data became available, see also Fig. 3. Despite the launch of the Sentinel-2A only in 2015, already 29 studies (5.1 %) made use of it for analysis (e.g., Abdi et al., 2021).

In Fig. 9d, trends in assessed aggregated land cover types of the reviewed studies are indicated. Category "Other" includes studies covering multiple land cover types as well as land cover/land use change studies. Hereby the dominance of agricultural studies can be clearly seen, followed by multiple, forests (e.g., Boisvenue et al., 2016) and finally grasslands (e.g., Brinkmann et al., 2011).

5.2 Agricultural applications

Exploration of TS data has been focused on cultivated areas due to the high significance of agroecosystems for providing global food security. In agricultural applications, grain or fruit yield is often considered the primary metric for productivity. Being indicated as "Vegetation Index" or "Traits" in Fig. 9a, these studies used VIs or quantitative traits as one of several inputs in data-driven or process models (e.g., He and Mostovoy, 2019; Ma et al., 2021; Guo et al., 2019) or transformed those into phenological metrics, such as calendar / thermal time or LoS (e.g., Duveiller et al., 2013; Azzari et al., 2017) to predict yield. With regards to VIs, mainly NDVI was used to predict crop yield (e.g., Lopresti et al., 2015; Suijker and Medrano, 2018). For instance, corn and soybean yield was estimated from six-year TS MODIS-driven NDVI by training regression tree-based models (Johnson, 2014) or for grape the yield was forecasted by training a separate artificial neural network with Landsat NDVI, LAI and normalized difference water index (NDWI) over three years (Arab et al., 2021). In a more complex set-up, Houborg et al. (2015) retrieved leaf chlorophyll content from Landsat TS data to constrain community land model simulations of GPP; whilst Yan et al. (2009) predicted the seasonal dynamics of GPP using a satellite-based vegetation photosynthesis model (VPM). The inclusion of multiple and heterogeneous data sources as inputs for ML models can improve results for crop yield forecasting. For instance, Perich et al. (2023) evaluated four different methods (including ML and deep learning) for pixel-based, within-field crop yield forecasts for five cereal crops from S2 time-series data across five years (2017–2021) and 54 fields. While their models showed good performance in general, the results also

demonstrated that the ability to predict yield for unseen years varied. This indicates that EO data alone might not be sufficient to explain complex productivity metrics such as yield. The importance of climate TS data, such as maximum temperatures and accumulated rainfall, along with EO data when training ML models was emphasised for crop yield forecasting by Kamir et al. (2020).

As a more direct proxy of plant photosynthetic activity, SIF may be able to directly indicate yield or agricultural production. The study by Somkuti et al. (2020), for instance, showed the potential of integrated GOSAT-derived SIF TS data to estimate crop yield. This research line of yield prediction has since then been adapted using other satellite sources of SIF (e.g. GOME-2, TROPOMI), thereby confirming that SIF contributes to improved yield prediction models (e.g., Peng et al., 2020; Sloat et al., 2021; Li et al., 2022).

5.3   Applications in forestry

In the last three decades, the bulk of research on forest productivity TS has focused on estimating AGB, and thus carbon sequestration, and better understanding the role of forests in regulating the climate. To accomplish these tasks, various types of data have often been combined, such as TS of satellite multispectral data (Landsat) with Light Detection and Ranging (LiDAR) and radar (e.g., Powell et al., 2010; Pflugmacher et al., 2014; Nguyen et al., 2020). The review by Nguyen et al. (2020) stated that innovative Landsat-based approaches for estimating forest AGB dynamics across space and time have been developed in recent years. Methods have become more advanced and robust over time. For instance, Landsat data can be used to fill in missing data points in AGB maps, which can improve the overall quality of the maps and make them more useful for applications such as carbon accounting and forest monitoring. Landsat data have been also used to estimate AGB over large areas and long time periods, even in areas where there is limited field data. Furthermore, recovery metrics can be used to improve the accuracy of AGB models since Landsat data can provide information about the dynamics of forests over time, which is not always captured by traditional AGB models.

Furthermore, forest disturbances can play a crucial role in ecosystem dynamics affecting productivity. Therefore, TS analysis of forest productivity is a fundamental tool for analyzing the magnitude and frequency of such events. Many of these forest disturbances are related and have increased due to climate change. Storms and forest fires have been highlighted as the most significant abiotic disturbances in Europe in recent years (Senf and Seidl, 2021). In addition, satellite TS analysis shows an increased trend in the frequency and intensity of droughts, and illustrative studies have been conducted for northern Europe (e.g., Reinermann et al., 2019; Senf et al., 2020; Descals et al., 2023). Climate change is also increasing the frequency of biotic disturbances like insect outbreaks (Senf et al., 2017; Olsson et al., 2017). Insect outbreaks in forests have a significant impact on productivity by defoliating trees and changing the structure of the forest. All these factors put our forests under increasing pressure and limit the forests' role as the global carbon sink. Therefore, it is essential to monitor temporal and spatial patterns of forest productivity by adopting suitable tools like EO data. To this end, many novel initiatives are related to this specific ecosystem. Examples are actions based on available data like the FAO's Global Forest Observations Initiative (GFOI) (Penman

et al., 2016). In recent years, the main concern about forest science has moved towards accurate carbon stock and
fluxes estimations, for which the focus on EO has shifted from multispectral proxy productivity estimations to precise
forest extension and AGB measurements, by means of LiDAR, radar, and SIF observations. Remotely sensed SIF
has become a widely used method to study temporal variations of deciduous and evergreen forests. In particular,
SIF retrieved from GOSAT (Lee et al., 2013), GOME-2 (e.g., Koren et al., 2018; Getachew Mengistu et al., 2021)
and TROPOMI (e.g., Doughty et al., 2019) was explored to study the relatively subtle seasonal variations in tropical
forests and provided new insights on vegetation activity during the transitions between wet and dry seasons.

5.4 Applications for natural ecosystems

For natural ecosystems, many studies assessed spatial and temporal trends in vegetation productivity for specific ecosystem types, often based on phenology indicators derived from TS of spectral VIs or by integrating those in DVMs. Among natural ecosystems, several studies focused on African semi-arid ecosystems (Sahel, South Africa) (Fensholt et al., 2013), the Arctic tundra (Beamish et al., 2020), the northern taiga (Canada, Alaska, Siberia, and Scandinavia) (Fiore et al., 2020) and the Middle-Asian grasslands, specifically in the Tibetan Plateau (You et al., 2019; Liu et al., 2020) and the Chinese-Mongolian area (Tüshaus et al., 2014; Gao et al., 2017). Regarding productivity, these studies assessed droughts, fires, changes in phenology metrics, land degradation, and vegetation mortality (e.g., Mayr et al., 2018; Buitink et al., 2020). The most used EO missions are MODIS and AVHRR, mainly through the analysis of NDVI and GPP TS, or to a lesser extent, other proxies (EVI, fAPAR) or metrics (NPP) of productivity (e.g., Rankine et al., 2017; Lara et al., 2018). The spatial coverage of these studies is global or regional, while the temporal extent is decadal, as MODIS and AVHRR cover a larger time period, from the 1980s to the present. Multiple studies took advantage of MODIS ready-to-use products (NDVI, EVI, fAPAR, GPP or NPP), which are compatible with specific phenology analysis software, see also Section 3.5. The MODIS GPP algorithms were also used in GPP estimation studies (e.g., Feagin et al., 2020) and for a comparison with a LUE-based DVM (Liu et al., 2011). Studies also compared the results of estimating GPP using MODIS and S2 TS data (e.g., Cai et al., 2021).

More recently, satellite SIF data became a valuable source for productivity estimations in natural ecosystems, among others to better capture seasonal periods of water stress and early-season GPP dynamics in drylands (Smith et al., 2018; Wang et al., 2019). Similarly, Merrick et al. (2019) studied satellite SIF data for different biomes, such as grasslands and savannas (among others). The authors concluded that the inclusion of SIF facilitated the differentiation of various vegetation types based on their functional characteristics and seasonal changes, explaining differences in year-round productivity dynamics. Despite being one of the most sensitive ecosystems, wetlands have been the least researched in the TS context, which might be due to their complexity. A few studies explored MODIS TS and EC flux tower data (e.g., Kang et al., 2018; Wang et al., 2021). Wang et al. (2021), for instance, used TS of the MOD17A3 annual NPP product to reveal spatial and temporal trends of NPP in China, among others. Analyses for wetlands are also oriented towards classifying changes in wetland extent on multi-temporal S2 imagery. Products

derived from multi-temporal data were used (S2, Landsat), like NDVI, for instance, to model NPP by means of the Carnegie-Ames-Stanford Approach (Zhang, 2021; Zhang et al., 2022a).

5.5 The role of productivity as a sink for carbon across ecosystems

Vegetation productivity, or GPP specifically, characterizes the "gross" terrestrial carbon sink, the gross amount of CO_2 annually sequestered by vegetation. NPP corresponds to the net carbon gain by plants, as it is the difference between the carbon produced by GPP and Ra (Fig. 10). The appropriation of NPP is also a measure of vegetation contribution to climate change mitigation (Alexandrov and Matsunaga, 2008). Overall, knowledge about the productivity of aboveground carbon stocks in forests, agriculture, and natural ecosystems is essential for global climate scenarios (Erasmi et al., 2021). Terrestrial ecosystems, along with the oceans, serve as a natural buffer that restricts the increase of CO_2 in the atmosphere by absorbing and sequestering nearly half of emitted CO_2 (Friedlingstein et al., 2022).

Fig. 10 delineates the different levels of productivity which are GPP, NPP, NEP, and NBP with respect to their carbon loss processes and flux densities over time. With increasing time scales, the four main fluxes are characterized by decreasing amounts of stored carbon due to diverse loss processes (GPP > NPP > NEP > NBP). Compared to GPP and NPP; NEP and especially NBP are relatively small (Watson et al., 2000). As denoted in Fig. 10, distinct ecosystems vary a lot in this respect. While an agricultural system (non-permanent crops) is releasing usually all carbon during one season, natural and forest ecosystems can store carbon for decades, depending on climate, but also on the amount of woody vegetation and tree age (Machwitz et al., 2015). This emphasizes the crucial role of TS data acquisition in monitoring the development of these carbon pools.

Due to the vast expansion of cultivated surfaces worldwide, the role of productivity of managed land within the global carbon cycle has also increased significantly and deserves particular dedication. Hereby, different factors have been found to influence the dynamics of carbon as sources or sinks, such as climate, tillage measures, fertilization or irrigation, among others (Luo et al., 2010). For example, tillage usually leads to a loss of soil organic carbon by organic decomposition, however, in combination and depending on other management practices a larger amount can be stored again by the crops (Haddaway et al., 2017).

The largest terrestrial carbon sink is the world's forests. In a general view, the global forest carbon stock in 2020 was 662 Gt (FAO, 2020), from which 44% is contained in the AGB. The tropics have the largest proportion of the world's forests, and hence they are highly relevant in terms of global climate regulation. However, tropical rainforests are under threat due to deforestation, logging, or cultivation, among others. These human activities lead to the loss of biodiversity and carbon storage, and thus to a transition of being carbon sources for the atmosphere. Also, other forest types play essential roles in this context, such as needle-leaf forest systems. A study in southern Sweden, for instance, focused on the plantation of needle-leaf trees (Grelle et al., 2023). The stands underwent a transition from positive (sources) to negative (sinks) annual carbon fluxes approximately 8 to 13 years after disturbance, influenced by site productivity and management, with net carbon gains of around 5 tC ha^{-1} year^{-1}. Additionally,

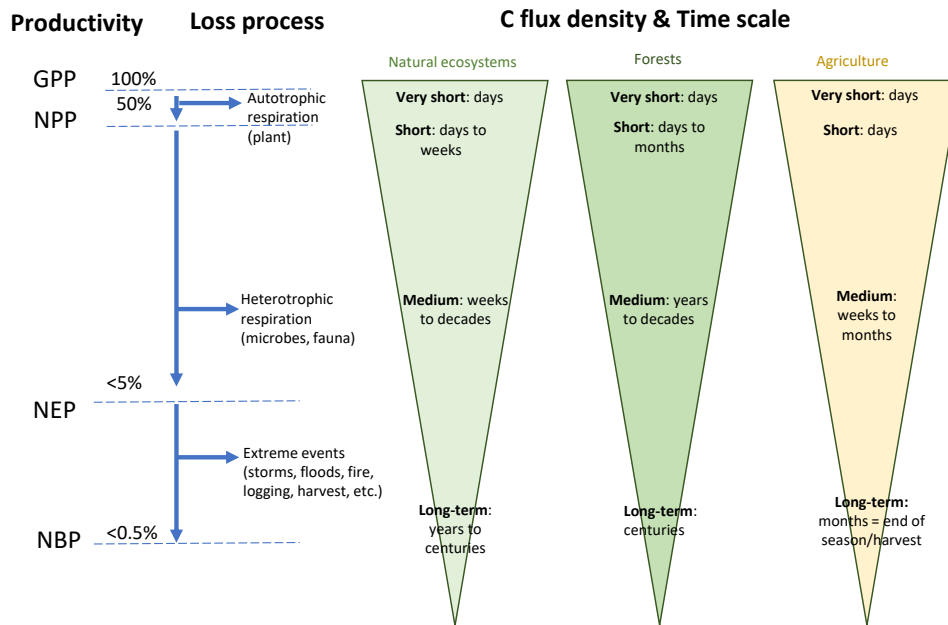



Figure 10. Overview of productivity terms along with their loss processes and C flux density over time scales and for the main ecosystems. Note that the given percentages are common average values and may vary.

tree crop-based agroecosystems, such as vineyards, have been linked to carbon storage facilities, with fixation rates up to 7.23 tC ha^{-1} year^{-1}, where the contribution of root systems implies 9-26% (Brunori et al., 2016) (which, however, cannot be quantified by EO techniques). A recent study on carbon density simulation in woody vegetation highlighted the need to advance model-data integration employing TS data streams, for a better understanding of the global terrestrial carbon cycle (Bultan et al., 2022).

6 Challenges and outlook

Our review revealed that multiple gaps, challenges, and opportunities exist to accurately estimate vegetation productivity from remotely sensed TS data streams. In this final section, we will discuss the main priority areas of research giving an outlook towards required efforts.

6.1 Key challenges

Efficient use of increasingly available and longer time-series datasets: Over the past few decades, there has been an increasing number of TS datasets made available, with enhanced spatial details as depicted in Fig. 3. Despite this progress, there may still be limitations in terms of the spatial and temporal resolutions for specific objectives and applications of monitoring vegetation productivity trends and processes. Some of these limitations include gaps in available long-term datasets due to persistent cloud cover, and discontinuity of sensors, leading to uncertainties in variable retrievals being relevant for vegetation productivity metrics. While with the advent of cloud-computing platforms access to EO data TS has never been as easy as nowadays, access to other RS resources (local airborne campaigns) is more fragmented and not always open. From a user's perspective, currently, there is a broad range of high-level, free and easy-to-use toolboxes available (as shown in Tab. 2), allowing and facilitating efficient TS processing.

Processes and factors affecting vegetation productivity: One important goal will be to adopt TS datasets to develop and test methods for heterogeneous natural environments, as the current focus is largely on croplands (see Fig. 9d). Satellite TS data streams can effectively capture, characterize, and quantify the spatiotemporal variation of natural processes. However, some approaches (discussed in Sect. 3) may only provide a relative characterization of vegetation productivity. To increase our understanding, process-based models (i.e., DVMs) are required to provide the mechanistic basis (linking to modelling domains) necessary to capture productivity variations in natural environments. Integrated modelling is a potential approach to address this need.

Availability of validation data and approaches: Effective validation of remotely sensed vegetation productivity products and derived productivity metrics is essential for ensuring their reliability and usefulness for a variety of applications. However, the collection of appropriate validation data (see Sect. 4), can be challenging for certain ecosystems. Moreover, there may be discrepancies in the terminology used by different scientific communities, which can hinder effective communication and collaboration. Thus, it is crucial to facilitate interdisciplinary exchanges to promote a common understanding of the terminology and concepts related to RS, as well as to foster collaborations that can help address knowledge gaps and advance the field.

Use of TS-based approaches to identify drivers of productivity change: TS-based approaches can be utilized to identify the drivers of productivity change, particularly concerning critical societal issues such as deforestation, land degradation, and climate change. Bultan et al. (2022), for instance, summarized that plant productivity has been underestimated using DVMs due to missing data from unprecedented extreme events, such as droughts. By providing a long-term perspective and enabling the detection of subtle changes over time, accurate TS data can help here and support more accurate predictions of future trends and impacts. Therefore, the use of TS-based approaches can play an important role in informing decision-making processes and promoting sustainable development.

Role for deep learning (DL) approaches to be adopted for explorative analysis and support system understanding: Classical RS data analysis methods for vegetation monitoring (including productivity studies)

usually require (manual) selection of appropriate features from the input data, for instance, spectral indices, texture metrics or temporal segments. The abundance of ways to derive such variables makes it difficult to find the most effective set of predictors for the automated identification of disturbances in vegetation productivity. Deep learning (DL) has been identified as a powerful method that can learn the most appropriate data transformations to get the most relevant data features for solving a specific problem (Kattenborn et al., 2021; Cherif et al., 2023). However, a key condition is the availability of a large training dataset, i.e., if the dataset is small, then conventional ML methods may be more suitable. For analysing data streams of temporal dynamics, recurrent neural networks (RNN) are of particular interest because they can recognize temporal patterns regardless of data gaps due to missing images or cloud cover. Similar to convolutional neural networks (CNN) for spatial patterns, RNNs make a selection of temporal features (e.g., trend, phenological indicators) obsolete (Kattenborn et al., 2021). A combination of RNN and CNN potentially enables an end-to-end processing scheme in the spatial and temporal domain and is considered by some authors a potential game changer in analysing TS data for vegetation applications such as productivity studies (Reichstein et al., 2019). Transformers are an alternative to RNNs that originate from natural language processing. Like RNNs, transformers are designed to process sequential input data, but unlike RNNs, they process the entire input all at once, which allows for more parallelisation and reduced training times. Very recently, transformers have started to advance into RS applications (Aleissaee et al., 2023).

6.2 Development of an integrated modelling approach towards the Digital Twin concept

We suggest that vegetation productivity research should focus on the integration of suitable multi-domain radiative transfer models (e.g. SCOPE) with process models (i.e., DVMs) (Moulin et al., 1998; Delécolle et al., 1992) to build Digital Twins of various ecosystems (Berger et al., 2022). This concept of real-time virtual representations allows us to mirror behaviour and states over the lifetimes of ecosystems and thus has the potential to overcome current limitations. Therefore, we should aim to develop a conceptual Digital Twin framework that implies a DVM with a fully integrated RTM for efficient vegetation productivity monitoring using RS TS data streams. Such integrated models directly simulate remotely observed signals based on the status of the underlying DVM at a point in time. This means the coupled DVM-RTM simulates the spectral signatures of the canopy (400 nm to 2500 nm) as well as SIF emission, along with physiological processes. To effectively assimilate the sensor data, it is necessary to create strategies that consider the varying availability of data from different sensors and sensor modalities over time. These strategies should enable continuous updates to the model, allowing for partial assimilation of variables while maintaining internal constraints and connections to additional variables.

Utilizing DVMs, which offer a continuous sequence of temporal growth dynamics, can be beneficial in identifying anomalies and enhancing the creation of continuous system descriptions. In this regard, incorporating a comprehensive numerical model, which assimilates such data, represents a significant advancement. Moreover, to accelerate the forward simulations, surrogate models or emulators can be used to replace some of the more intricate models (Verrelst et al., 2019b). Since DVMs are partly driven by weather variables, they may also allow the integration

of weather forecasts and/or climate scenarios in such model designs. This dynamic nature would meet the requirements of a Digital Twin of ecosystems, which besides the representation of the current status, also predicts their future behaviour (Verdouw et al., 2021).

7   Conclusions

Monitoring vegetation productivity is critical for understanding the health and functioning across ecosystems. In recent years, the increasing availability and quality of optical TS data streams resulted in a large-scale use for monitoring vegetation productivity metrics (e.g. GPP, NPP, crop yield or AGB) for a range of application domains adopting both RS-derived phenological indicators and increasingly more complex integrated modelling approaches. In this review, we identified a vast number of studies that used remotely sensed TS data streams and distinct methods for inferring productivity metrics. These efforts led to valuable insights into vegetation dynamics across ecosystems, including agriculture, forests, grasslands, and others. As the perhaps most urgent topic nowadays, spatially explicit estimating vegetation productivity is crucial for understanding the role of ecosystems in the carbon cycle. By using satellite data to estimate the amount of carbon stored in vegetation, we can better understand the impact of land use changes (e.g., deforestation) and other human activities on the global carbon balance, and thus climate change. The availability of long-term satellite TS data streams with improved spatial and temporal detail has increased steadily over the past decades. More recently, the emergence of routinely acquired SIF products proved to provide a more direct linkage towards photosynthetic activity and became increasingly integrated into vegetation productivity processing chains. Validation efforts in ensuring the accuracy, robustness, and reliability of RS-based productivity estimates are another essential aspect of the processing chains. Validation can be performed in several ways, including *in situ* measurements, local sensor networks, and inter-comparisons of available productivity products or models. The definition of harmonized validation strategies is critical to ensure that the methods used to infer productivity from EO data are robust and accurate across various ecosystems and conditions. It also provides confidence in the data and models used to inform management decisions and climate change mitigation strategies. Additionally, we foresee that due to the advancements in artificial intelligence, the processing approaches of TS data streams will diversify, and at the same time, the modelling approaches will significantly advance towards holistic processing and representations of vegetation productivity. Our proposed conceptual framework of a Digital Twin aims to address the limitations of existing approaches and may provide more accurate and efficient productivity estimation supporting the management of ecosystems at varying scales.

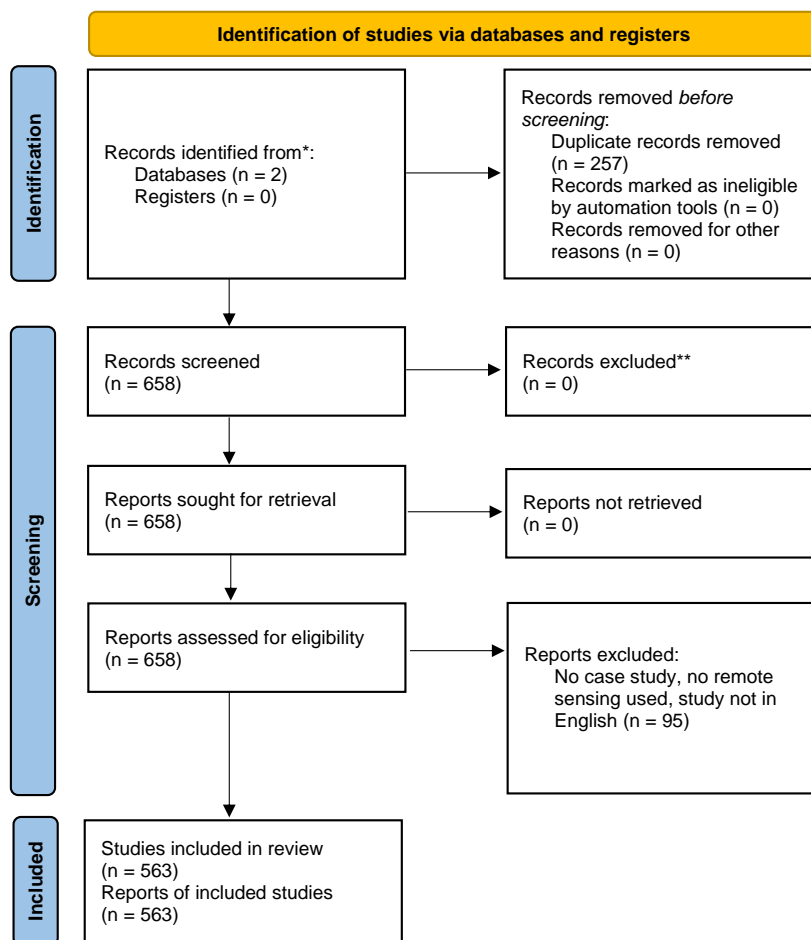



Figure A1. Identification of studies via databases and registers according to PRISMA (Page et al., 2021).

Appendix A

Author contributions. Conceptualisation: LK, KB, MM, MS, BB, JV, HA; Formal analysis: BB, DG, ET, FF, GK, IH, LK, LG, MK MR, MM, OR, RD, SRK, VEG; Investigation: KB, JV, ET, MR, MM; Methodology: LK, KB, HA, JLR, LVG, BB, JV; Software: KB, EP, JV; Supervision: LK, KB, JV, HA, JLR; Visualization: DG, MM, PRM, MS, KB, AH, BB; Writing - original draft: LK, KB, JV, HA, JLR, MM, LVG, BB, CA, VGM, EP, GK, BB, ET, OR, MS, SB, CSF, SRK, PRM; Writing - review and editing: LK, KB, MM, MS, JV, HA, JLR, ZC, LVG, MR, MK, SC, GK, VGM, JP, HC, ETG, MK.

Competing interests. TEXT

Herewith we declare that no competing interests are present.

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