



UNIVERSITÀ DEGLI STUDI DI NAPOLI
FEDERICO II

DEPARTMENT OF BIOLOGY

National PhD Program in Artificial Intelligence for Agrifood and Environment

Thesis for the Degree of Doctor of Philosophy

Inference of Water Deficit Indices of Crop and Vegetation from Satellite Hyperspectral Infrared Sensors

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Academic Year: 2024/2025

Cycle: XXXVIII

Abstract

Global warming is intensifying extreme weather events worldwide, amplifying droughts, floods, and wildfires. In 2024, the global mean temperature reached 1.55 ± 0.13 °C above pre-industrial levels, surpassing the Paris Agreement threshold. Among all climate-related hazards, drought is one of the most complex phenomena and also one of the most difficult to define and monitor. Assessing drought events is crucial and satellite observations can provide significant support thanks to their large spatial coverage and continuous data supply.

Vegetation is often among the first systems to exhibit stress because of its high sensitivity to water availability. However, since drought events generally cover vast areas, vegetation monitoring has to be done remotely, traditionally through Vegetation Indices (VIs). VIs describe remotely sensed vegetation properties such as photosynthetic activity, canopy structural variations and water content. In this context, a new Water Deficit Index (WDI) was introduced, defined as the linear difference between the Land Surface Temperature (LST) and the Dew Point Temperature (T_d). This index gives a compact and physically interpretable measure of surface heating relative to ambient dryness and has already proven effective in detecting water stress in plants. The computation of the index is straightforward, but the retrieval of the required variables is more complex. Specifically, the retrieval of remotely sensed T_d is the most challenging. Unlike LST, which is a radiometric “skin” property that can be derived from a few Thermal Infrared (TIR) channels, T_d is an atmospheric parameter typically obtained from vertical profiles, thus requiring hyperspectral infrared sensors.

Thanks to its high spectral resolution, the Infrared Atmospheric Sounding Interferometer (IASI) is the only sensor capable of simultaneously retrieving LST, T_d , and several other atmospheric parameters. IASI combines excellent spectral and temporal resolution (8461 channels and two overpasses per day per platform) with a spatial resolution of approximately 12 km at nadir. These characteristics have enabled the development of a retrieval scheme that simultaneously estimates the LST, the full emissivity spectrum, vertical profiles of temperature, water vapour, and ozone mixing ratio, as well as atmospheric trace gases concentrations and, as indirect products, the relative humidity and T_d . The complete forward/inverse processing chain for IASI data is implemented in a software package called ϕ -IASI, a FORTRAN-based inverse radiative transfer code for the optimal estimation of the thermodynamic state of the atmosphere. The retrieval scheme was tested over two Italian regions: the Po Valley region (northern Italy) and Basilicata region (southern Italy).

Unfortunately, the retrieval of geophysical parameters from IASI radiances is limited by the nature of the sensor. Since IASI is a TIR sounder, it cannot penetrate thick cloud layers (clouds are opaque in the TIR), resulting in reliable retrievals only for clear-sky pixels. This introduces

missing data, requiring an interpolation step to transform the sparsely populated, non-uniform Level 2 (L2) observations into evenly-gridded maps Level 3 (L3).

In this work a downscaling–fusion methodology was applied. Several Machine Learning (ML) algorithms with complementary strengths have been explored, including Random Forest (RF), Gradient-Boosted Trees (GBT), Neural Network (NN), and Gaussian Process Regression (GPR), and Stacked Regression. Specifically, the models were developed to predict LST and T_d at the locations of the L2 satellite observations, using a set of covariates derived from other satellite sensors, vegetation products, reanalysis datasets, and territorial and geographical information. All input datasets were spatially and temporally co-located with the L2 observations to ensure consistency. Subsequently, the predicted LST and T_d fields were downscaled by exploiting the higher spatial resolution of the covariates, producing estimates over a regular 0.05° grid, thereby effectively doubling the spatial resolution of the original data.

From the downscaled L3 LST and T_d , the WDI was computed, and its robustness was assessed by validating LST and T_d individually. Validating LST products is challenging because only a few ground stations exist worldwide. Given the strong spatial heterogeneity of LST, the evaluation focused on the method’s ability to capture finer details and small variations in LST at the target resolution. In this context, the L3 outputs were compared against the LST from the Moderate Resolution Imaging Spectroradiometer (MODIS). Conversely, T_d validation was carried out using data from the regional Agenzia Regionale per la Protezione dell’Ambiente (ARPA) network, which provides reliable in situ observations across Italy. Results indicated that the downscaling–fusion methodology significantly improved spatial sampling, while maintaining very low errors. Specifically, the comparison with MODIS for LST and the validation against ARPA stations for T_d showed a better agreement for the L3 product than for the L2, confirming that the enhanced spatial resolution effectively captured the underlying spatial variability. The ability of the WDI to capture plant water deficits was further confirmed by comparison with other remotely sensed water stress indicators, namely the Normalized Difference Moisture Index (NDMI) and Surface Soil Moisture (SSM).

Finally, the focus shifted towards the projections of the WDI. Understanding how vegetation water stress may evolve under climate change requires more than a snapshot of recent events. It is important to identify long-term trends and determine whether it is becoming a more frequent event. Future climate projections provide a key tool for this analysis. However, since most future projections are based on precipitation-based indices, WDI-based projections provide additional value by offering a complementary perspective. To project the WDI, an ensemble of 13 EURO-CORDEX simulations was used, considering both an intermediate (RCP 4.5) and a worst-case (RCP 8.5) scenario. The analysis focused on the Italian peninsula and was subsequently restricted to the Po Valley and Basilicata regions. The projections indicated consistent positive WDI anomalies across Italy in all seasons and under both scenarios, suggesting an increase in water stress. These anomalies are particularly pronounced in the Po Valley, the islands, and Basilicata, especially under the worst-case scenario.

The work developed in the present thesis has been published in:

- Italia De Feis, Fabio Della Rocca, Giuliano Liuzzi, Guido Masiello, Pamela Pasquariello, and Carmine Serio. Retrieval of surface and atmospheric parameters from high resolution infrared sensors. *Mathematics and Computers in Simulation*, 239:950–966, 2026. (Chapters 5 and 3)
- Fabio Della Rocca, Pamela Pasquariello, Guido Masiello, Carmine Serio, and Italia De Feis. Machine learning to retrieve gap-free land surface temperature from infrared atmospheric sounding interferometer observations. *Remote Sensing*, 17(4), 2025. (Chapters 3 and 4)
- Fabio Della Rocca, Italia De Feis, Guido Masiello, Pamela Pasquariello, and Carmine Serio. Comparison of the IASI water deficit index and other vegetation indices: the case study of the intense 2022 drought over the Po Valley. In Adolfo Comerón, Evgueni I. Kassianov, Klaus Schäfer, Richard H. Picard, and Konradin Weber, editors, *Remote Sensing of Clouds and the Atmosphere XXVIII*, volume 12730, page 127300C. International Society for Optics and Photonics, SPIE, 2023. (Chapters 3 and 4)
- Fabio Della Rocca, Italia De Feis, Guido Masiello, Pamela Pasquariello, and Carmine Serio. Machine learning techniques for spatial interpolation of the IASI water deficit index. In Evgueni I. Kassianov and Simone Lolli, editors, *Remote Sensing of Clouds and the Atmosphere XXIX*, volume 13193, page 1319307. International Society for Optics and Photonics, SPIE, 2024. (Chapters 3 and 4)

An article derived from Chapter 5 is currently in preparation.



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List of Acronyms

The following acronyms are used throughout the thesis.

ABI	Advanced Baseline Imager
ARPA	Agenzia Regionale per la Protezione dell’Ambiente
ASTER	Advanced Spaceborne Thermal Emission and Reflection Radiometer
AVHRR	Advanced Very-High-Resolution Radiometer
CWSI	Crop Water Stress Index
CLC	CORINE Land Cover
CMIP	Coupled Model Intercomparison Project
CMK	Contextual Mann–Kendall
CNN	Convolutional Neural Network
CORDEX	Coordinated Regional Climate Downscaling Experiment
DBSCAN	Density-Based Spatial Clustering of Applications with Noise
DEM	Digital Elevation Model
ECMWF	European Centre for Medium-Range Weather Forecasts
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
ET	Evapotranspiration
FAPAR	Fraction of Absorbed Photosynthetically Active Radiation
FDR	False Discovery Rate
FOR	Fields Of Regard
FOV	Field Of View
FVC	Fraction Vegetation Cover
GBT	Gradient-Boosted Trees
GCOS	Global Climate Observing System

GCM	Global Climate Model
GEE	Google Earth Engine
GHG	Greenhouse Gas
GOES	Geostationary Operational Environmental Satellites
GP	Gaussian Process
GPR	Gaussian Process Regression
IASI	Infrared Atmospheric Sounding Interferometer
IASI-NG	IASI Next Generation
IQR	Interquartile Range
IPCC	Intergovernmental Panel on Climate Change
IR	Infrared
IRS	Infrared Sounder
KDE	Kernel Density Estimate
LAI	Leaf Area Index
L1	Level 1
L2	Level 2
L3	Level 3
LSE	Land Surface Emissivity
LSA SAF	Satellite Application Facility on Land Surface Analysis
LST	Land Surface Temperature
MAE	Mean Squared Error
MetOp	Meteorological Operational
MIR	Mid-Infrared
MK	Mann–Kendall
ML	Machine Learning
MODIS	Moderate Resolution Imaging Spectroradiometer
MW	Microwave
NASA	National Aeronautics and Space Administration
NDMI	Normalized Difference Moisture Index
NDVI	Normalized Difference Vegetation Index

NIR	Near Infrared
NN	Neural Network
NOAA	National Oceanic and Atmospheric Administration
NWP	Numerical Weather Prediction
PCA	Principal Component Analysis
PC	Principal Component
RCM	Regional Climate Model
RCP	Representative Concentration Pathway
RF	Random Forest
RMSE	Root Mean Square Error
RTE	Radiative Transfer Equation
SE	Squared Exponential
SEVIRI	Spinning Enhanced Visible and Infrared Imager
SPI	Standardized Precipitation Index
SPEI	Standardized Precipitation–Evapotranspiration Index
SSM	Surface Soil Moisture
SST	Sea Surface Temperature
SSP	Shared Socioeconomic Pathway
SW	Split-Window
SWIR	Shortwave Infrared
T_d	Dew Point Temperature
TES	Temperature and Emissivity Separation
TIR	Thermal Infrared
TIRS	Thermal Infrared Sensor
VCTFPW	Variance Corrected Trend Free PreWhitening
VI	Vegetation Index
VIS	Visible
VPD	Vapor Pressure Deficit
WDI	Water Deficit Index
XGBoost	eXtreme Gradient Boosting

Chapter 1

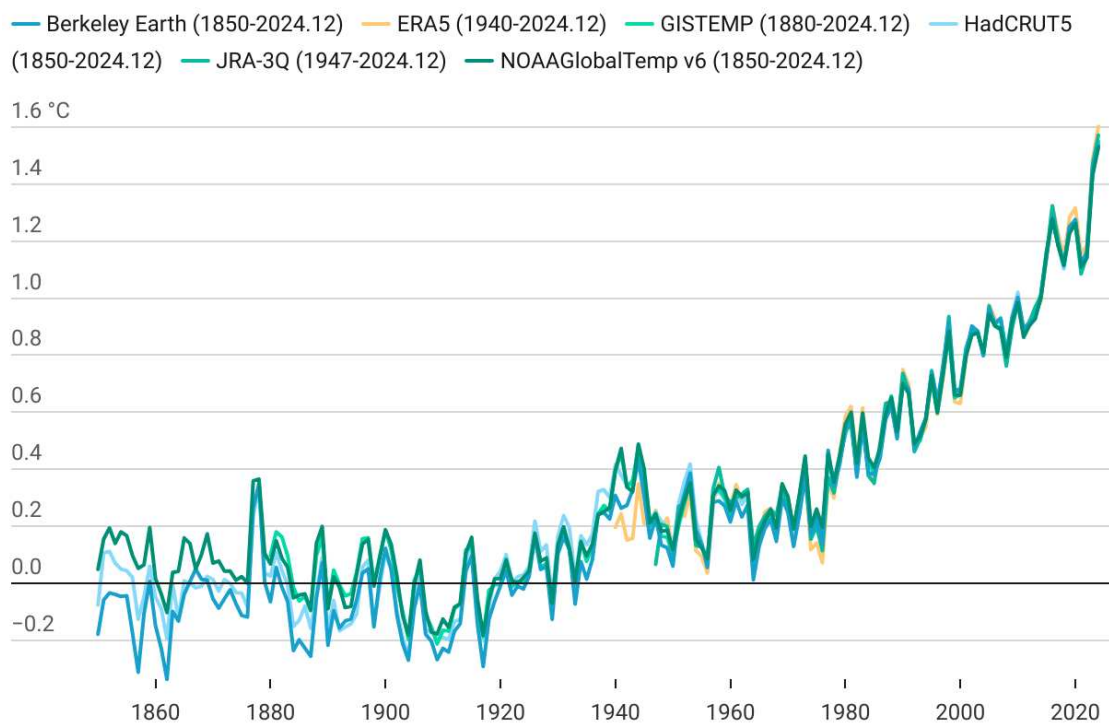
Drought Monitoring: From Concepts and Indices to the Water Deficit Index

1.1 Introduction

Global climate change is widely recognised as a major driver of the increasing frequency and intensity of extreme events. Rising global temperatures are making already dry regions drier, and wet regions wetter, leading to a range of severe phenomena as floods, tropical storms, hurricanes but also droughts, wildfires, and desertification. Year after year, new climate records continue to be broken. In 2024, for the first time, the average global temperature reached 1.55 ± 0.13 °C above the pre-industrial level (1850-1900), surpassing the limit established by the Paris Agreement [241]. This marks the warmest year in the 175-year instrumental record. The previous record year, 2023, exhibited an anomaly of 1.45 ± 0.12 °C above the pre-industrial baseline [240]. However, a single year with an anomaly higher than 1.5 °C does not imply that the long-term target of the Paris Agreement has already been breached. Global temperature does not rise uniformly year after year as a substantial interannual variability is present. Volcanic activity, changes in ocean circulation, and phenomena such as El Niño and La Niña contribute to variations between individual years. According to the IPCC, the time of crossing a warming level is defined as the midpoint of the first 20-year period (or, alternatively, a 10-year period) during which the average global surface temperature exceeds that level [110]. Nevertheless, the evidence confirms that the warming trend is clear and persistent, as illustrated in Figure 1.1.

Global mean temperature 1850-2024

Difference from 1850-1900 average



Annual global mean temperature anomalies relative to a pre-industrial (1850–1900) baseline shown from 1850 to 2024

Chart: WMO • Created with Datawrapper

Figure 1.1: Annual global mean air temperature anomalies (at 2 m) relative to a pre-industrial (1850–1900) baseline shown from 1850 to 2024. Source: WMO [241]

Europe remains the fastest warming continent, experiencing temperature increases at approximately twice the global average rate. The continent continues to break temperature records: the three warmest years ever recorded in Europe have all occurred within the last five years, with the last one being the year 2024 [40].

Among all climate-related hazards, drought is one of the most complex phenomena and also one of the most difficult to define and monitor. It can be described as a period of time when an area or region experiences drier than normal conditions, typically characterised by a significant decrease in precipitation relative to the historical average. In contrast to rapid-onset events such as floods, storms, or wildfires, drought develops slowly and often goes unnoticed until its impacts become severe, accumulating over months or even years. For this reason, it is often referred to as a *creeping phenomenon* [75]. Unlike aridity, which represents a permanent climatic condition, drought is a temporary but recurrent meteorological event that can occur virtually everywhere, from arid deserts to humid tropics.

According to Wilhite and Pulwarty, “drought is an insidious natural hazard that results from a deficiency of precipitation from average or ‘normal’ that, when extended over a season or

longer, results in water supplies insufficient to meet the demands of human activities and the environment” [239]. A deficit in precipitation is the primary trigger of drought events, but it is not the only contributing factor. Other meteorological and environmental variables, such as low humidity, strong winds, and particularly high temperatures, also play a crucial role in determining the severity and duration of a drought episode. Due to the complexity of the phenomenon, no universally accepted definition of drought exists. Instead, definitions must be contextualized according to the specific application domain, as the impacts of drought vary considerably depending on whether the focus is on agriculture, water resources, or ecosystems.

This has led to the identification of several drought categories, which are summarized in Table 1.1.

Table 1.1: Summary of the main types of drought, with their definitions and degree of human interaction.

Type of Drought	Definition and Focus	Human Interaction
Meteorological	Defined in terms of a precipitation deficit over an extended period of time. Represents the beginning of the drought process.	Determined mainly by natural climatic factors.
Agricultural	Occurs when there is not enough moisture in the soil to sustain the growth of crops.	Influenced by soil management practices, soil properties (e.g., water-holding capacity), irrigation practices.
Hydrological	Results from prolonged meteorological and agricultural drought. Leads to reduced surface and sub-surface water availability.	Strongly influenced by the use and management of surface and groundwater resources (e.g., irrigation, hydropower generation).
Socioeconomic	Occur when water supply is too low to support human and environmental needs, affecting economic sectors or social groups. It is of particular interest to policymakers.	Strongly influenced by water and land management policies as well as demand dynamics (e.g., population growth).

For instance, the absence of adequate precipitation (meteorological drought), whether in the form of rain or snow, can lead to reduced soil moisture and groundwater levels, diminished stream flow (hydrological drought), crop damage (agricultural drought), and an overall shortage of water resources (socioeconomic and environmental drought). Additional factors, such as high temperatures, low humidity, and strong winds, further exacerbate the intensity and duration of drought events. Figure 1.2 illustrates the typical sequence of drought development and the

corresponding impacts across different drought categories.

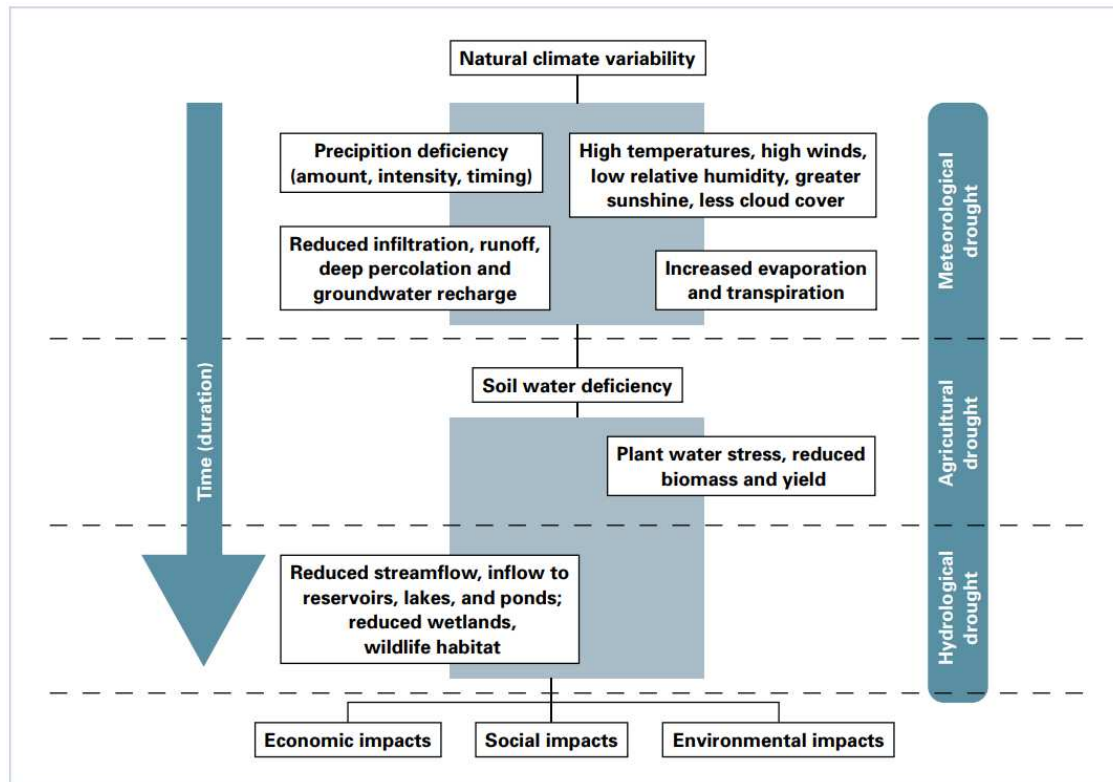


Figure 1.2: Sequence of drought occurrence and impacts for drought types. All droughts originate from a precipitation deficit (meteorological drought) from which other drought types and their associated impacts develop over time. Source: WMO [243]

Nevertheless, it is important to identify long-term trends and assess whether droughts are becoming more frequent events, as they are contributing, together with desertification, increasing agricultural demands and land degradation, to a growing global water crisis. In particular, drought has severe impacts in semi-arid regions and Mediterranean mid-latitudes: in forested areas, prolonged drought conditions can substantially increase the risk of wildfire, whereas, in semi-arid zones, drought primarily results in pronounced water stress. The wide range of sectors affected by drought, combined with the strong spatial and temporal variability of its characteristics, highlights the need for multiple indicators capable of capturing the various types and manifestations of drought.

The growing exposure of natural and human systems to drought hazards amplifies overall risk, making it essential to monitor key characteristics such as onset, duration, intensity, and spatial extent to support effective risk assessment and forecasting [228, 140]. Drought monitoring relies on the use of indicators and indices that capture variation in the regional water cycle. The **indicators** describe drought conditions through variables such as precipitation, temperature, streamflow, groundwater, reservoir and lake levels, soil moisture, and snowpack. The **indices**, on the other hand, are numerical representations derived from these indicators, providing quantitative

measures that describe the severity, spatial extent, timing, and duration of drought events.

In the early days, drought monitoring relied exclusively on precipitation measurements [90]. However, the development of drought indices, i.e., mathematical formulations that integrate multiple variables into a single quantitative metric, has provided a more robust and comprehensive representation of drought conditions than the use of individual variables alone [4]. The earliest drought indices were based solely on precipitation data from gauges. Examples include the Rainfall Anomaly Index (RAI) (1965)[230], the Deciles Index (DI) (1967)[73], the Effective Drought Index (EDI) (1999)[25], among others.

The Standardized Precipitation Index (SPI) [158] is the most widely adopted drought index. It indicates the deviation of precipitation from the climatological mean over a specified accumulation period. Nevertheless, the inherent complexity of drought necessitates consideration of additional variables beyond precipitation alone. Therefore, a comprehensive assessment requires the incorporation of data on temperature, evapotranspiration, river flow, and soil moisture [4, 121, 183, 147]. Examples include the Palmer Drought Severity Index (PDSI) [181] and the Standardized Precipitation–Evapotranspiration Index (SPEI) [231], which also account for temperature and evapotranspiration, respectively. Historically, such indices relied solely on **weather station data**, which were subsequently interpolated onto a regular grid. While effective for characterising temporal anomalies, these traditional methods exhibit several known limitations: their accuracy and representativeness are contingent upon station density and quality control; they often fail to capture local heterogeneity; and they do not directly reflect the physiological response of vegetation [244, 219]. Crucially, these indices are confined to addressing precipitation deficits, thus characterising only **meteorological drought**. Recent technological advances in **satellite imagery**, however, have enabled the combination of a wide array of drought-related indicators. This allows for the creation of composite indices that incorporate the specific environmental or ecological characteristics of a given region.

1.2 Beyond Precipitation: Towards Multi-Variable Drought Indices

Vegetation is often among the first systems to exhibit stress because of its high sensitivity to water availability. Plants respond to **water deficits** through a plethora of physiological and structural changes, including stomatal closure [67, 227, 89], reduced photosynthetic activity [67], loss of turgor [14], increases in canopy temperature [112, 81], and, in severe cases, irreversible damage or mortality. These responses make vegetation a valuable indicator of drought conditions, as it integrates the combined effects of meteorological and hydrological anomalies over time and space.

Compared to meteorological and hydrological indices, the development of agricultural drought indices remains limited [4]. These specialized indices shift the focus from precipitation to variables like Evapotranspiration (ET) and soil moisture. They are typically categorized according to their dominant input: soil moisture–based, evapotranspiration–based, and vegetation–based indices.

Soil moisture-based drought indices use estimates of volumetric soil water content or soil water anomalies to quantify plant-available water in the root zone. Examples are the Crop Moisture Index (CMI) [182], the Soil Water Deficit Index (SWDI) [149], the Soil Moisture Deficit Index (SMDI) [173], the Soil Moisture Anomaly Index (SMAI) [19], among others.

Drought conditions typically involve coincident meteorological factors—namely, elevated air temperatures, lower humidity, and stronger solar radiation—that collectively drive increased ET. As ET integrates both water availability and atmospheric demand, **evapotranspiration-based** drought indices are highly effective at capturing drought development, particularly under hot, dry conditions. Examples include the Evapotranspiration Deficit Index (ETDI) [173], and the DTx index [157]. Some indices are crop-specific, as they account for plant responses to drought, such as the Crop Specific Drought Index (CSDI) [164] for corn (*Zea mays L.*) and the Soybean Drought Index (SDI) [163] for soybean (*Glycine max*).

Vegetation-based indices describe the actual performance of plant canopies, providing a direct measure of biological response rather than merely reflecting atmospheric conditions. They assess stress based on changes in greenness, canopy structure, surface temperature, and plant water content due to water stress. Since physiological changes often precede visible damage (e.g., leaf browning or stunted growth), vegetation-based indices can offer an earlier indication of drought stress compared to metrics based solely on climatic factors. However, they are an indirect measure of drought, since they quantify stress on plants. It is important to note that plant stress is not exclusively caused by drought, as reduced vigour or leaf yellowing can be induced by various factors. These include biotic factors (insect pests, diseases, competition with other plants) and abiotic factors (extreme temperatures, **drought**, salinity, heavy metals, and floods) that induce reduced vigour or leaf yellowing. Nonetheless, vegetation effectively integrates the combined effects of weather, soil, and crop–water management (e.g., irrigation scheduling, cultivar choice, tillage). By reading the plant signal, researchers can determine the **actual** impacts of drought, rather than focusing solely on meteorological forcing. In the context of drought monitoring, vegetation indices should therefore assess anomalies relative to local climatology and be verified against meteorological or hydrological evidence (e.g., SPI/SPEI, soil moisture, ET).

1.3 Remote Sensing and Vegetation Indices

The high spatial resolution, ease of use, free access, and global coverage contribute to the proliferation of a multitude of vegetation indices based on spectral reflectance/emission in the Visible (VIS), Near Infrared (NIR), Shortwave Infrared (SWIR) (≈ 400 nm to 2500 nm), and Thermal Infrared (TIR) (≈ 8 μ m to 14 μ m). The vegetation typically absorbs in the red and blue wavelengths, reflects in the green, strongly reflects in the NIR, and displays strong absorption features in wavelengths where atmospheric water is present (SWIR)(see Figure 1.3). Vegetation monitoring has traditionally been accomplished through Vegetation Indices (VIs), which describe remotely sensed vegetation properties such as photosynthetic activity and canopy structural variations. Vegetation-

based indices can be grouped by their primary remote sensing signal into three families, each possessing distinct strengths and weaknesses: **canopy water content**, **thermal/energy balance**, and **greenness**.

- The **canopy water content** family uses the NIR–SWIR contrasts to track changes in leaf and canopy water status. Indices such as Normalized Difference Moisture Index (NDMI) [28], Leaf Water Content Index (LWCI) [102], or Normalized Multi-band Drought Index (NMDI) [237] are more closely correlated with plant water content and can respond earlier than greenness alone. However, since stress in plant canopies can be caused by factors other than drought, isolating drought-specific effects using only these indices remains challenging.
- The **thermal/energy balance** family of indices exploits the physical relationship between water stress and reduced transpirational cooling. Specifically, stomatal closure reduces the cooling effect provided by transpiration, consequently increasing the canopy temperature. These thermal approaches are highly advantageous, as they can detect drought stress in plants approximately **2–3 weeks before visual symptoms**, such as leaf desiccation [81]. These indices are generally based on canopy temperature or Land Surface Temperature (LST), computed from TIR data. Examples include the Temperature Condition Index (TCI) [125], the Crop Water Stress Index (CWSI) [106], the Normalized Difference Temperature Index (NDTI) [160], among others. However, thermal methods also face inherent challenges. They require reliable atmospheric and emissivity corrections [45] and careful attribution of temperature increases, as canopy temperature can rise due to high air temperature even in well-watered conditions, leading to potential confusion with heat waves that lack moisture limitations [146].
- The **greenness** indices measure vegetation greenness, reflecting both chlorophyll content and leaf area. This approach relies on the principle that chlorophyll strongly absorbs red light, while healthy leaves exhibit high scattering in the NIR. Normalized Difference Vegetation Index (NDVI) [199], the most widely used vegetation index, is a classic example that exploits this difference. In addition to the red and NIR bands, the Enhanced Vegetation Index (EVI) [99] also includes the blue band to reduce atmospheric aerosol effects and better characterise canopy structure. Other examples include the Ratio Vegetation Index (RVI) [117], the Vegetation Condition Index (VCI) [125], and the Soil-Adjusted Vegetation Index (SAVI) [100]. This family also includes Fraction of Absorbed Photosynthetically Active Radiation (FAPAR). FAPAR is an indicator that measures the state and photosynthetic activity of vegetation by quantifying the fraction of Photosynthetically Active Radiation (400 nm to 700 nm) that is absorbed. FAPAR values, and especially their anomalies, have been shown to be effective indicators for detecting and assessing drought impacts on plant canopies [78].

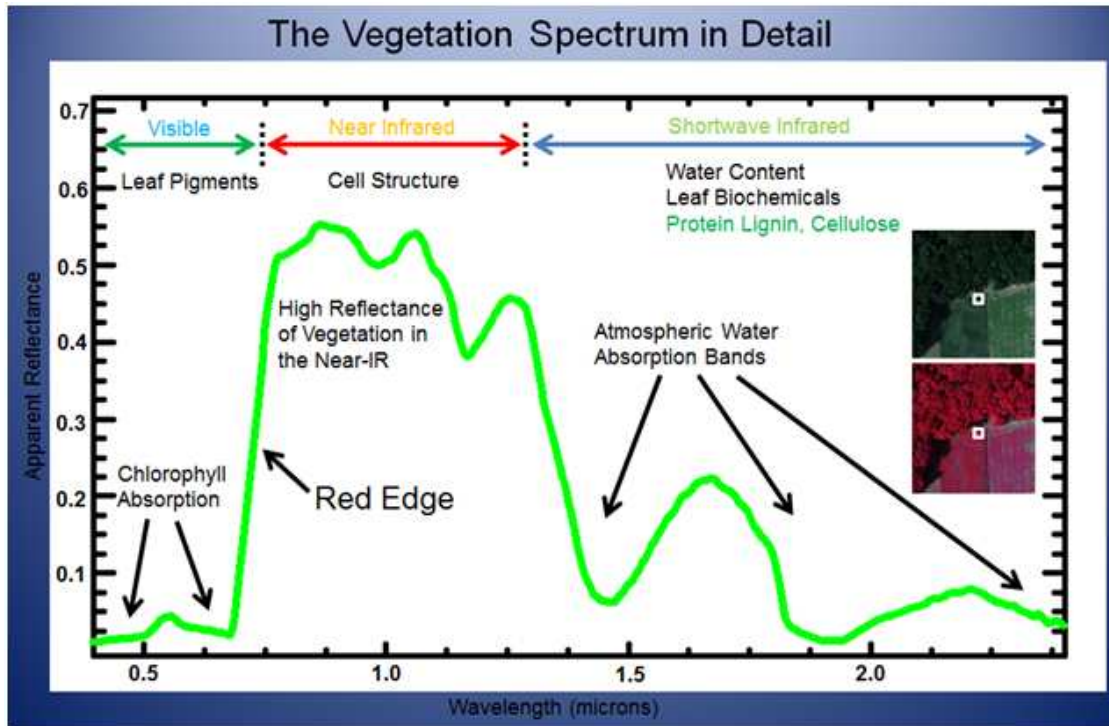


Figure 1.3: Vegetation reflectance spectrum showing chlorophyll absorption in the visible, the near-infrared red edge, and water absorption features in the shortwave infrared, which form the basis of many vegetation indices. Source: NV5 [177]

Other indices are of **integrated type**, such as the improved Temperature Vegetation Dryness Index (iTVDI) [248], which integrates LST and NDVI, or the Soil Moisture Agricultural Drought Index (SMADI) [220], which integrates LST, NDVI and soil moisture. However, the problem with NDVI-like indices is that they are greenness indices and cannot distinguish bare soil from senescent vegetation, yet this distinction is essential, especially when dealing with semi-arid regions. Indeed, in these regions the soil background can affect NDVI, as decreasing vegetation cover makes the signal increasingly contaminated by soil reflectance [101, 232]. Moreover, neither LST nor air temperature is directly linked with soil moisture and inconsistent results have been found in some specific situations (e.g., [118]).

Despite its utility, the TIR spectral region has only been marginally exploited, even though spectral emissivity in this range is highly sensitive to surface type and soil moisture. Furthermore, the retrieval of the atmosphere's thermodynamic state and near-surface hydrometeorological conditions from TIR data can be directly related to surface evapotranspiration. TIR observations provide direct evidence of reduced transpirational cooling, while near-surface humidity serves as a comprehensive summary of both atmospheric demand and the resulting evapotranspiration rate. These two signals can be effectively combined into a simple measure of water deficit that is independent of vegetation greenness and robust over sparse canopies.

1.4 The Water Deficit Index (WDI)

The **Water Deficit Index (WDI)** is an index proposed by Masiello *et al.* in 2022 [151, 209] and defined according to the linear difference between the Land Surface Temperature (LST) and the Dew Point Temperature (T_d) as follows:

$$WDI = LST - T_d. \quad (1.1)$$

LST and T_d are two fundamental parameters that characterise the water exchanges between the surface and the atmosphere. Their combination can be related to the surface evapotranspiration.

The conceptual foundation for indices relating surface temperature to plant water stress is well-established in the literature. This concept was principally formalized by Idso and Jackson (1981) with the introduction of their CWSI [106, 112]. They demonstrated that the difference between canopy temperature (which approximately corresponds to LST areas completely vegetated) and air temperature has a **linear relationship** with the air Vapor Pressure Deficit (VPD). Moran *et al.* (1994) [169], extended the CWSI theory to partially vegetated fields using composite surface temperatures and spectral vegetation indices. This work highlighted the critical role of surface-air temperature differences as key indicators of plant water status. Considering canopy rather than air temperature is particularly important when characterising the effects of compound heat and water stress. This approach also helps assess mitigating potential of irrigation against heat stress, as canopy temperature can be substantially higher than air temperature under water stress [146]. This concept was later improved in [151, 209], where T_d was used instead of air temperature to better represent the effect of atmospheric humidity. T_d acts as an observational proxy of atmospheric moisture (and thus VPD, which is a function of air temperature and T_d), so $LST - T_d$ gives a compact, physically interpretable measure of surface heating relative to ambient dryness. This formulation offers a crucial advantage: during heat waves with humid air (high T_d), the WDI remains low, limiting false drought detections due to heat alone; conversely, in hot-dry conditions (low T_d), the WDI rises, accurately capturing the severity of drought stress.

As discussed earlier, a precipitation deficit is not always an indicator of plant water stress. During photosynthesis, plants use sunlight, water (taken from the soil) and carbon dioxide (absorbed from the atmosphere) to produce glucose and oxygen. Water uptake occurs via the roots, while the exchanges with the atmosphere, including the absorption of carbon dioxide and the release of oxygen, are regulated by small aperture on the leaves called stomata. Through this process, known as transpiration, plants also lose water. Transpiration allows plants to cool down (crucial during summer) and drives the absorption and transport of water and nutrients from the soil via a water potential gradient. Stomatal closure is the earliest response to drought and the dominant limitation to photosynthesis at mild to moderate drought [67]. Similar to mammalian sweating, transpiration cools plants in a process that involves the vapourization of liquid water in plant tissues and the consequent release of vapour into the atmosphere. During this phase change, from liquid water to gas, an amount of heat (latent heat of evaporation) is lost from the

evaporating surface, cooling down the vegetation. However, the cooling effect is determined by the availability of soil moisture in the root zone and plants prevalent environmental condition.

Nearly all water taken up by a plant is lost through transpiration, with only a tiny fraction being used within the plant. Transpiration, much like direct evaporation, depends on the energy supply, vapour pressure gradient at the surface–atmosphere interface, wind, and soil water content [6]. A satellite-based index that aims to quantify water deficit, as the WDI, should consider solar radiation, air temperature, air humidity, wind velocity and soil water content [151]. In Eq. (1.1), the energy supply is represented by LST, as solar radiation drives a rapid rise in the surface temperature. Meanwhile, T_d reflects both air temperature and air humidity. While incorporating the effect of wind is more challenging, droughts and heatwaves conditions are often characterised by air subsidence and weak pressure gradients, hence reducing the impact of the wind.

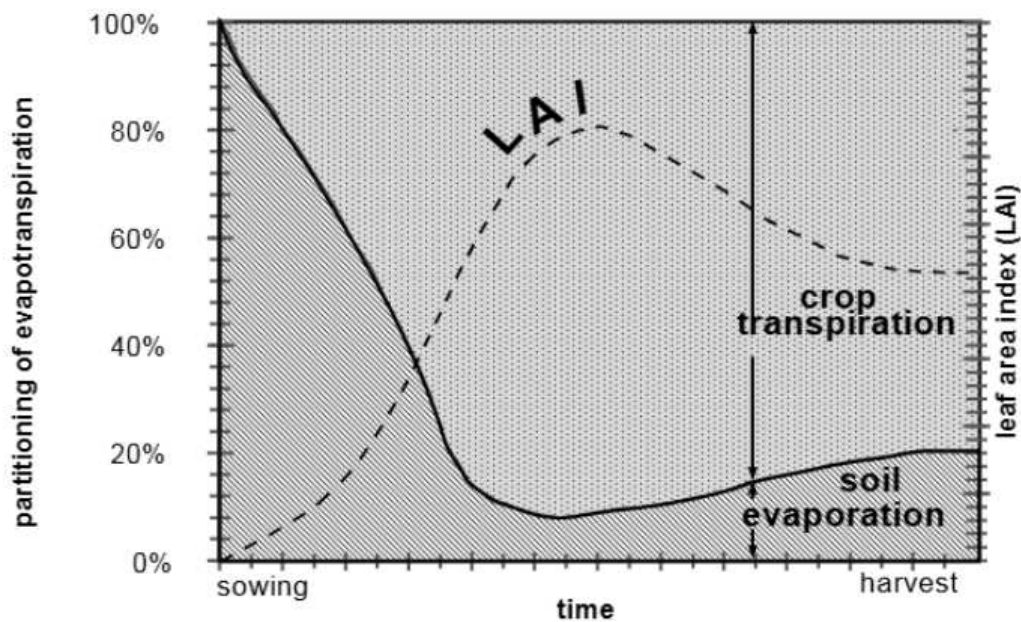


Figure 1.4: The partitioning of evapotranspiration into evaporation and transpiration over the growing period for an annual field crop. Source: Allen *et al.* (1998) [6]

It is also important to note that evaporation and transpiration occur simultaneously, and distinguishing between these two processes is often difficult. As depicted in Figure 1.4, evaporation dominates when the vegetation is sparse, allowing more solar radiation to reach the soil, while transpiration is the main process in well-developed crops that completely cover and shade the soil. For this reason, we employ the term evapotranspiration (the sum of the two processes) when referring to the total water exchange between the land surface and the atmosphere.

Because the WDI is more closely related to surface type, canopy coverage, and soil moisture, it effectively aids in understanding water stress during droughts or heatwaves. Specifically, it assesses the vegetation water deficit and facilitates a better separation of a hot-dry ($WDI \gg 0$) from a humid-warm (WDI approximately equal to zero) weather condition. The WDI generally

increases when canopies (and surfaces) warm due to reduced transpiration (i.e. a reduced cooling effect) and when the air is dry (i.e. low T_d or, equivalently, high VPD). This behavior is consistent with the well-established thermal rationale for plant water stress: lower stomatal conductance reduces latent heat flux, thereby raising canopy temperature (which approximately corresponds to LST of fully vegetated areas). Unlike other vegetation indices, the WDI does not have a strictly defined fixed range of values (e.g. -1 to +1 for the NDVI), nor does it come with an interpretation guide for its values (e.g., 0.2 to 0.5 of NDVI values meaning sparse vegetation). As it represents a difference of temperatures, its unit is still degrees (Celsius or Kelvin), and its values exhibit clear seasonal variability. However, despite the lack of a fixed range, a qualitative interpretation of the values can still be provided. For example, an high WDI during summer results not only from hotter weather but also from a reduction in water vapour exchange between the surface (such as soil and vegetation) and the atmosphere. Indeed, if the soil is already dry less evaporation occurs and the plants close their stomata limiting the transpiration [67, 227, 89]. A reduction in transpiration means less gaseous exchanges between plants and the atmosphere, limiting photosynthetic activity, and thus plant growth. Conversely, a WDI close to zero represents a humid condition where the evapotranspiration rate is low, and the vapour condenses in liquid water at the surface (dew). Dew plays an important role in the water cycle between the air and land surface [167, 258]. In arid and semi-arid regions such as the Mediterranean area, dew is a major factor affecting vegetation water use efficiency: even if it seems that dew can be insufficient as a source of water for plants, it creates a humid environment close to the leaf, minimizing transpiration during stomata aperture, maximizing carbon intake [15] thereby promoting healthy plant growth. Although exact thresholds separating optimal/non-optimal conditions depend on vegetation and surface type, for forests and cultivated green areas in temperate climates, a WDI of 4-8 °C is considered optimal. Values below 3 °C indicate air that is too humid, increasing risks of condensation and pathogens, while values above about 10 °C reflect very dry air and potential plant water stress due to stomatal closure. (see, e.g. [80, 136]).

WDI has already been shown to be a good indicator of **vegetation water deficit** in forests during droughts. For example in [151], WDI was compared against in situ observations for the flux exchange of CO₂ and H₂O from *Quercus frainetto* trees. The authors found that higher WDI values corresponded to higher water vapour exchange and lower photosynthetic water-use efficiency. This confirms the relationship between WDI and evapotranspiration, as well as its connection to plant water stress.

1.5 How to Retrieve WDI

The WDI index is a simple index based solely on two variables: LST and T_d . The computation of the index is straightforward, but the retrieval of the required variables is more complex.

1.5.1 Land Surface Temperature

Land Surface Temperature (LST) refers to the radiative skin temperature of the land (soil or top of the canopy) and can be described as a measure of how hot or cold the surface of the Earth would feel to the touch [82]. LST is one of the 55 Essential Climate Variables, a group of linked variables that critically contributes to the characterisation of Earth's climate defined by a panel of experts from the Global Climate Observing System (GCOS). Its importance covers many fields such as meteorology, climatology, agriculture, evapotranspiration, urban planning, and environmental monitoring [137].

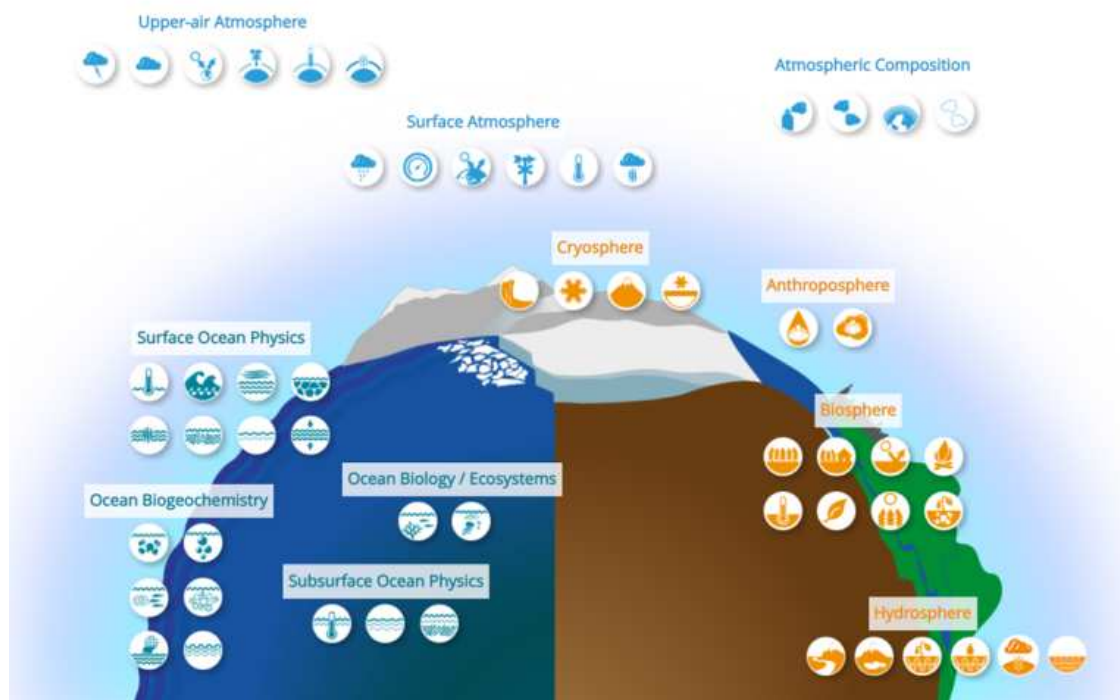


Figure 1.5: Diagrammatic representation of the 55 Essential Climate Variable identified by GCOS. Source: GCOS [71].

We can have two LST products: in situ observations and remotely sensed products. In situ observations are primarily used for validation and calibration of satellite-based LST data, rather than as standalone products. This is because LST is highly variable depending on surface materials, vegetation cover, soil moisture, atmospheric conditions, and topography, which can make in situ measurements less representative on larger scales. TIR or Microwave (MW) remote sensing is considered to be the most efficient way to obtain accurate LST, both regionally and globally. However, as in all remotely sensed products, there is a trade-off between spatial, spectral, and temporal resolution. For example, TIR images from Moderate Resolution Imaging Spectroradiometer (MODIS), have a high temporal resolution (twice a day) but a relatively coarse spatial resolution (1 km). Other sensors such as the Thermal Infrared Sensor (TIRS) onboard LANDSAT platforms, have a greater spatial resolution (100 m in this case) but much lower temporal resolution (8 days). In contrast, TIR images from geostationary satellites, like from

Spinning Enhanced Visible and Infrared Imager (SEVIRI), have a much lower revisit time (minutes) but at the cost of low spatial resolution (≈ 5 km). Having a coarse resolution, results in the thermal mixture effect, i.e., when a given thermal pixel contains a blend of multiple thermal signals that are smaller than the resolution cell [257]. Therefore, there is a growing need to improve the spatial resolutions of LST products.

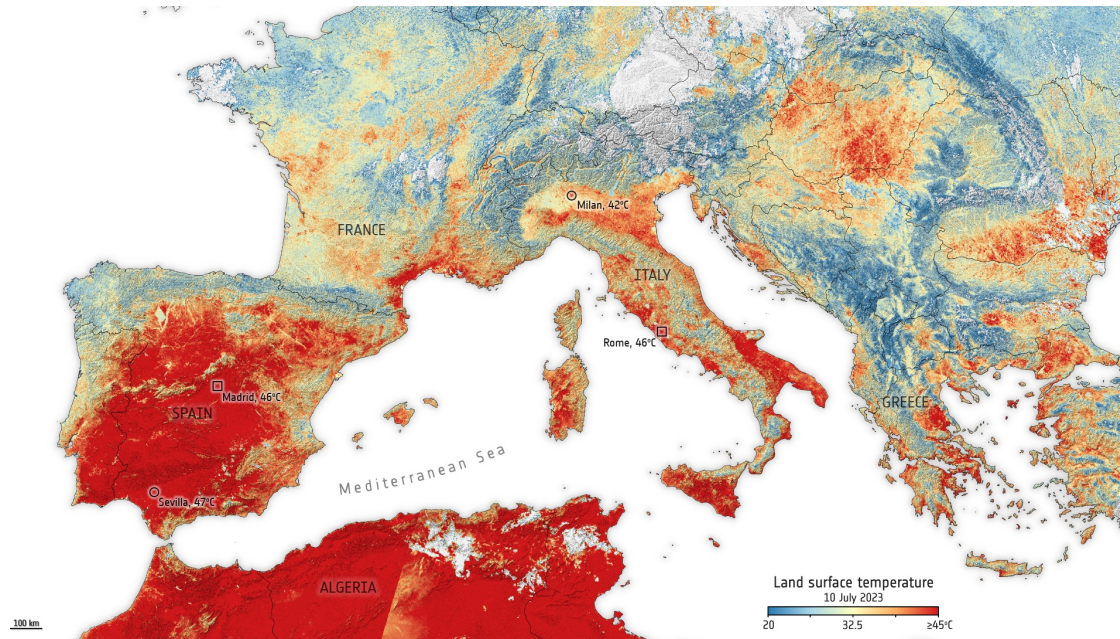


Figure 1.6: Example of LST across Europe on 10 July 2023 retrieved from Copernicus Sentinel-3. In some cities the LST exceeded 45 °C, including Rome, Madrid, and Seville. Source: ESA [65].

The LST retrieval commonly relies on one or more channels within the TIR region, spanning $8\mu\text{m}$ to $13\mu\text{m}$. This interval, known as the **infrared atmospheric window**, is a portion of the infrared spectrum where atmospheric gases absorb relatively little terrestrial thermal radiation, allowing the atmosphere to be more transparent. This window plays a crucial role in the atmospheric greenhouse effect by maintaining the balance between incoming solar radiation and outgoing infrared radiation to space. Satellite sensors take advantage of this window to retrieve LST with minimal atmospheric distortion. These channels also correspond to the wavelengths of the peak monochromatic radiance, predicted by Wien's displacement law, for typical LST values (ranging from approximately 250 K to 330 K). The retrieval of LST from TIR radiances is a physical process that involves the inversion of the Radiative Transfer Equation (RTE). However, estimating LST from satellite-measured radiance requires corrections for both atmospheric and emissivity effects, which is a challenging task. The inversion of the RTE is an underdetermined and ill-posed problem [94, 120], even when atmospheric parameters are known, for N channels there are still $N + 1$ unknowns (N emissivities and the LST, which is independent of wavelength). To make the retrieval of LST a deterministic problem, it is necessary to know the value of at least one emissivity in advance. Alternatively, the LST and Land Surface Emissivities (LSEs) can be estimated simultaneously by imposing physical assumptions or constraints on

the LSE [137, 94, 120, 42, 74]. Numerous algorithms have been proposed for estimating LST from satellite observations, which can be broadly classified into three categories: single-channel algorithms, multi-channel methods, and multi-temporal methods [138]. The single-channel method [191, 116, 115] is the simplest approach, relying on the inversion of the radiative transfer equation, provided that LSEs and atmospheric profiles are known in advance. Multi-channel methods include the Split-Window (SW) algorithm and the Temperature and Emissivity Separation (TES) method. Among these, the SW algorithm is the most commonly used for LST retrieval from satellite data and takes advantage of the differential atmospheric absorption in two adjacent TIR channels [159]. Examples of LST products generated using an SW algorithm include MODIS LST (MOD11) from the National Aeronautics and Space Administration (NASA) [235], VIIRS (Visible Infrared Imaging Radiometer Suite) LST from the National Oceanic and Atmospheric Administration (NOAA) [142], Sentinel-3 LST from the Copernicus Sea and Land Surface Temperature Radiometer (SLSTR) [72], GOES LST from the Advanced Baseline Imager (ABI) onboard NOAA's Geostationary Operational Environmental Satellites (GOES) [253], and LST products from the Satellite Application Facility on Land Surface Analysis (LSA SAF) derived from SEVIRI and AVHRR sensors [225]. However, this method still requires the LSEs to be known a priori, and LST retrieval accuracy is degraded under a highly humid atmosphere or at large viewing zenith angles [138, 36, 55, 251]. An improvement over the SW algorithm is provided by the TES algorithm [74], which utilises multiple TIR channels and an empirical relationship between the minimum LSE and the difference between maximum and minimum LSE to dynamically retrieve both LST and emissivity. An example of its application is NASA's LST MOD21 product from MODIS [174]. However, the performance of the TES performance is limited by the accuracy of the atmospheric correction, and the results can be inaccurate for surfaces with low spectral emissivity contrast (i.e., similar emissivity in different channels), such as dense vegetation, water, and snow [138]. Multi-temporal methods combine multi-temporal information under the assumption that LSEs do not change significantly between adjacent day and night observations. For example, the physical day and night algorithm [236] employs both TIR and Mid-Infrared (MIR) bands to accurately retrieve LST and LSE in a physical way. However, the retrieval is complicated by the fact that two clear, independent, and perfectly co-registered observations are needed. Additionally, it still requires an a priori approximate atmospheric profile, and it assumes constant emissivity throughout the day, which may not be true (e.g., due to condensation or dew formation).

1.5.2 Dew Point Temperature

The **Dew Point Temperature** (T_d) is the temperature to which air must be cooled at constant atmospheric pressure and constant water vapour content for saturation to occur. It is computed from air temperature and relative humidity. A simple approximation is given by Eq. (1.2):

$$T_d \approx T - \frac{100 - RH}{5}, \quad (1.2)$$

where T is the air temperature ($^{\circ}\text{C}$) and RH is the relative humidity (%). In practice, T_d rises when the air mass is humid and drops when it is dry, becoming equal to the air temperature when the relative humidity reaches 100%. For example, as illustrated in Figure 1.7, a condition of 21°C and 50% RH (indicated by the blue cross) yields a T_d of approximately 10°C . Conversely, maintaining the same air temperature but increasing the humidity to 75% would result in a T_d of approximately 15°C (not shown in the figure).

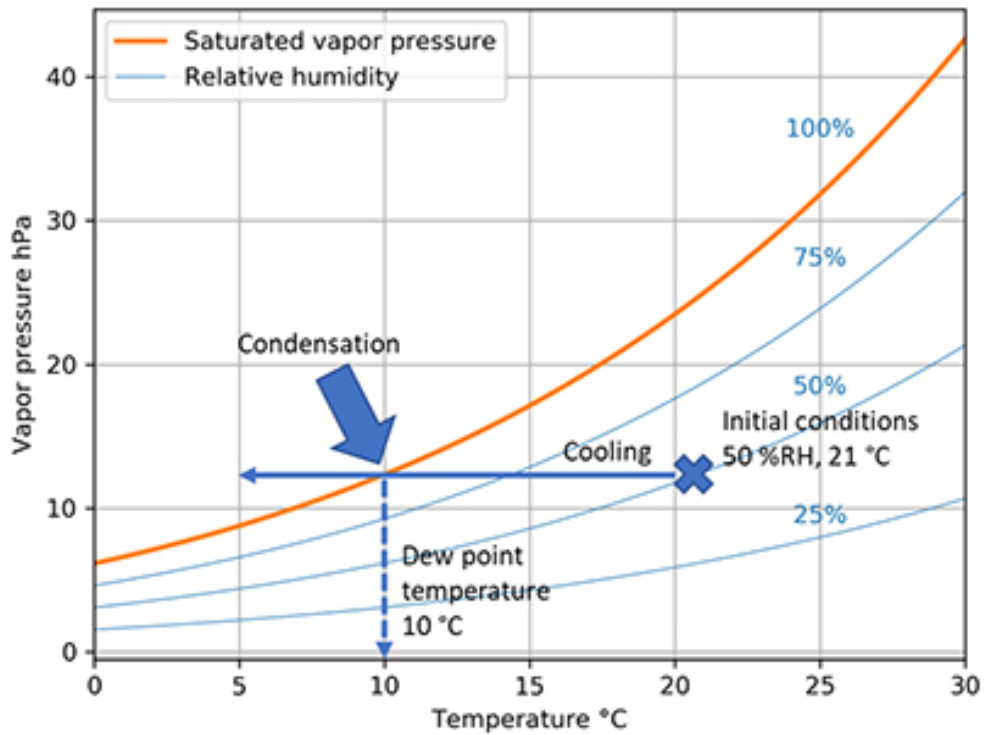


Figure 1.7: Chart explaining the relationship between air temperature, relative humidity and dew point temperature. X-axis: air temperature ($^{\circ}\text{C}$); y-axis: vapour pressure (hPa); orange curve: saturated vapour pressure (hPa); blue lines: relative humidity (RH) isolines (%). For example, the marked example starts at 21°C , 50% RH . Cooling at constant vapour pressure moves left horizontally until it meets the orange curve at about 10°C , that is the dew point temperature. Source: Vaisala [184].

Water vapour itself is one of the Essential Climate Variable in the GCOS framework, emphasising the climatic importance of near-surface humidity metrics such as T_d .

We can distinguish between two primary T_d products: in situ observations and remotely sensed products. Unlike LST, in situ T_d is a more commonly available product, with most of the T_d maps derived from weather stations. These stations compute T_d from standard 2-m observations of air temperature and RH using well-established psychrometric relations (e.g., Magnus equation). These station observations are often interpolated onto a regular grid. An example is E-OBS[27], a

daily gridded land-only observational dataset covering Europe. However, T_d observations are typically available only from a limited number of weather stations, often irregularly distributed, and interpolation techniques can reduce the spatial representativeness.

On the other hand, remotely sensed T_d is less straightforward to obtain. Satellites do not retrieve T_d directly: it must be computed from its constituents air temperature and RH . These variables are generally retrieved as **profiles** from which the near-surface equivalent can be derived. Unlike LST, these are not radiometric “skin” properties, but atmospheric variables. Retrievals are generally based on hyperspectral Infrared (IR) sensor (limited to clear-sky conditions), sometimes coupled with MW sensors, which provide complementary information from the lower atmosphere in cloudy pixels.

The most widely used product is the **European Centre for Medium-Range Weather Forecasts (ECMWF) reanalysis ERA5** and its spatially enhanced version, **ERA5-Land**. Reanalyses datasets combine a Numerical Weather Prediction (NWP) model with data assimilation of diverse observations (including satellite radiances, radiosondes, and surface weather stations) to provide gap-free, physically consistent fields at regular temporal and spatial resolutions. However, a known limitation of these products is their relatively coarse spatial resolution (0.1° for ERA5-Land), which may not adequately capture local-scale variability, especially in regions with complex topography such as Italy.

MODIS delivers global, high-quality observations of land surface and atmospheric parameters, offering a valuable alternative to characterise fine-scale T_d variability over large areas. Although MODIS is not a hyperspectral sounder and lacks stratospheric channels, NASA adapted the International TOVS Processing Package (ITPP) [213] to compute the MODIS Atmosphere Profile (MOD07_L2 for Terra platform and MYD07_L2 for Aqua platform). The algorithm [203] computes the clear-sky profiles using a two-step scheme: first a statistical regression (based on [212]) is applied to the radiances in order to get a first guess of the atmospheric profiles; then a non-linear iterative physical algorithm (based on [132]) is applied to the RTE to improve the solution. This product provides, in addition to total ozone burden, atmospheric stability, and atmospheric water vapour, both temperature and moisture profiles distributed across 20 vertical levels, which enable the computation of T_d at a spatial resolution of 5 km. However, MODIS remains a multispectral instrument providing only a limited number of broad spectral bands and thus limiting its ability to retrieve atmospheric vertical profiles. Indeed, a recent study validating near-surface MODIS T_d against ground-based observations over mainland China reported a general Root Mean Square Error (RMSE) exceeding 5°C [262].

1.5.3 LST and T_d retrieval from the Infrared Atmospheric Sounding Interferometer (IASI)

In this thesis the retrieval of both LST and T_d from spaceborne observations for the computation of the WDI was carried out using data from , onboard the Meteorological Operational (MetOp) series of polar-orbiting satellites. Thanks to its high spectral resolution, IASI is the only sensor capable of simultaneously retrieving the LST, the emissivity spectrum, and atmospheric composition,

overcoming the limitations of previous approaches. IASI combines excellent spectral and temporal resolution with a spatial resolution of approximately 12 km at nadir. These characteristics have enabled the design of a retrieval scheme that simultaneously estimates the LST, the complete emissivity spectrum, the vertical profiles of temperature, water vapour, and ozone mixing ratio, as well as the atmospheric concentration of trace gases and, as indirect products, the relative humidity and T_d .

The retrieval scheme was tested over the following two target area: Po Valley and Basilicata region. The interaction among the different components of the research is illustrated in Figure 1.8.

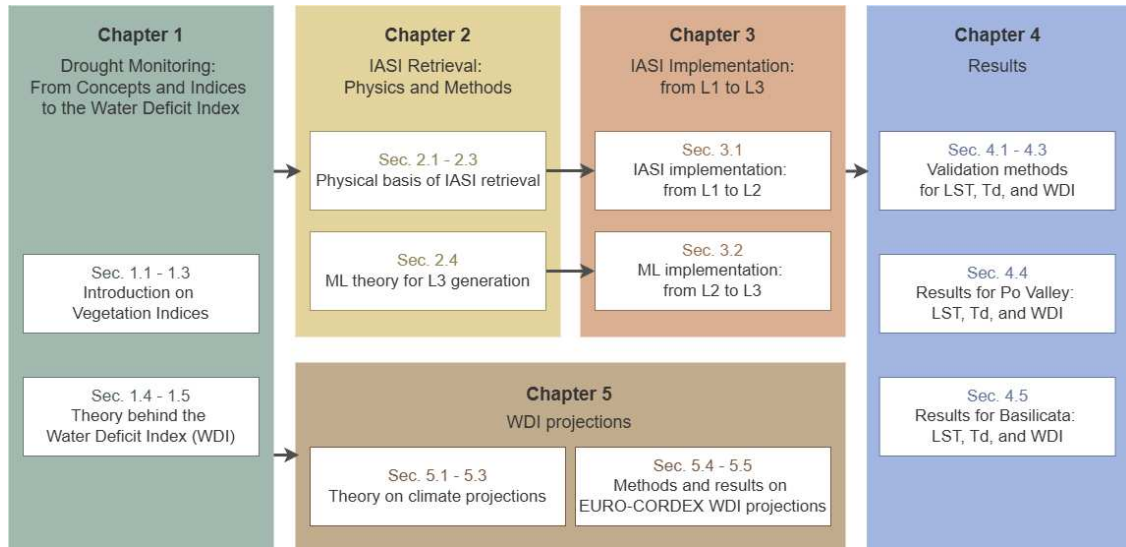


Figure 1.8: Overview of the research workflow, from the conceptual introduction to the WDI to the IASI retrieval framework, the machine learning–based downscaling approach, and the WDI climate projections.

Chapter 2 introduces the physical and theoretical foundations of the IASI retrieval, along with the theoretical framework of the machine learning methods adopted for downscaling and gap-filling. Chapter 3 describes the implementation of the retrieval of the geophysical parameters (L2) from IASI radiances and the machine learning approach used to produce gap-filled and downscaled products (L3). Chapter 4 presents the results of the LST, T_d , and WDI retrievals for the two target regions. Finally, Chapter 5 discusses the climate projections and the corresponding WDI results.



Chapter 2

IASI Retrieval: Physics and Methods

2.1 IASI Instrument

IASI [92] is a Fourier transform spectrometer that measures infrared radiation emitted from the Earth. IASI was developed in France by the Centre National d'Etudes Spatiales (CNES) and is flying on board the MetOp platforms, satellites of the European Polar System (EPS) operated by European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT). In total, three MetOp platforms have been launched, MetOp-A, MetOp-B and MetOp-C. The first was launched on 19 October 2006, the second on 17 September 2012, and the last on 7 November 2018. The three satellites were originally intended to be operated sequentially, each with a design lifetime of five years. However, due to the longer than expected in-orbit performance of MetOp-A and MetOp-B, all three MetOp platforms were operated simultaneously. Currently, MetOp-B and MetOp-C are still operational, while MetOp-A was decommissioned in November 2021 (with the last IASI scene recorded on 15 October 2021) [63]. Figure 2.1 shows the temporal coverage of IASI data for the three MetOp platforms (data taken from [49] and [62]). The satellites have a

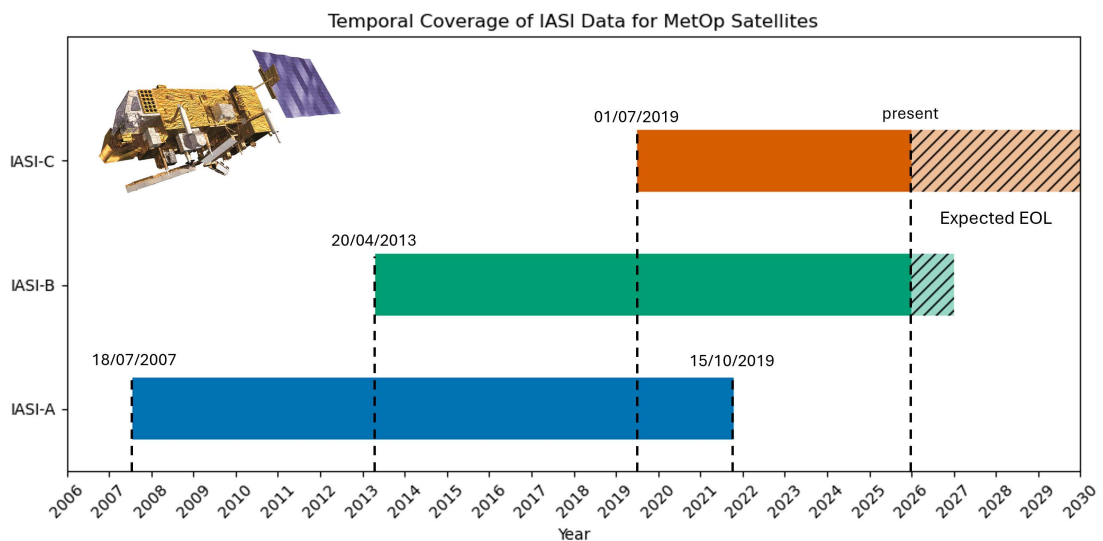


Figure 2.1: Temporal coverage of IASI data for the three MetOp platforms.

sun-synchronous orbit at an altitude of around 817 km with a 98.7° inclination to the equator. The satellite's ground track is at about 09:30 local time in the morning and 21:30 in the evening. With a swath width on the Earth's surface of 48.3° on both sides of the satellite track (2200 km in total), global coverage is achieved in 12 hours, hence providing a day and night passage. The time to complete an orbit is about 101 min, which implies that MetOp makes slightly more than 14 orbits per day.

IASI is a cross-track scanner with 30 adjacent Fields Of Regard (FOR) per scan. Each FOR covers a square area of $50 \times 50 \text{ km}^2$ on the ground and consists of a 2×2 matrix of instantaneous fields of view (IFOVs) with a diameter of 0.8394° (corresponding to a ground resolution of 12 km at nadir). The spectral coverage of the instrument extends from 645 cm^{-1} to 2760 cm^{-1} with a spectral sampling of 0.25 cm^{-1} providing a total of 8461 channels. The effective spectral resolution is 0.5 cm^{-1} due to Gaussian apodization. Figure 2.2 shows an example of a IASI spectrum, with the main absorption bands. The 8461 spectral samples are aligned in 3 bands within the spectral range,

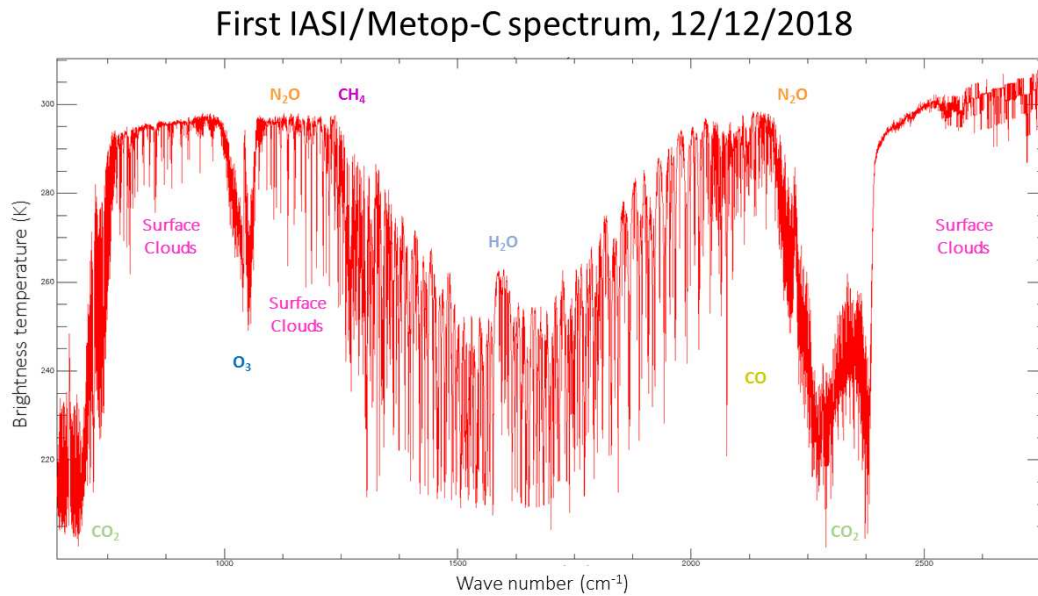


Figure 2.2: The first spectrum from the IASI instrument on board Metop-C. Source: www.eumetsat.int/metop-cs-iasi-instrument-delivers-first-spectrum

as shown in Table 2.1. Although primarily intended to provide information in near real-time

Table 2.1: Definition of IASI bands		
Band Number	Wavenumber (cm^{-1})	Wavelength (μm)
1	645 - 1210	8.26 - 15.50
2	1210 - 2000	5.00 - 8.26
3	2000 - 2760	3.62 - 5.00

on atmospheric temperature and water vapour to support weather forecasting, the instrument can also retrieve concentrations of various trace species, as well as surface parameters, from the

spectra.

Before describing the methodology employed to retrieve the main atmospheric components from IASI radiances, it is necessary to provide a detailed explanation of the typology of the satellite products. In the terminology of satellite observations, we distinguish between Level 1 (L1), Level 2 (L2) and Level 3 (L3) data (see <https://osi-saf.eumetsat.int/about/acronyms>). L1 refers to radiances, which are the direct measurements from the instrument. L2 refers to geophysical parameters obtained using suitable retrieval schemes from L1 observations. L2 data are sparse, and the sparseness depends on the spatial density and distribution of clouds and, to a lesser extent, the time slots dedicated, e.g., to instrument calibration. L3 products are derived from L2 products on a regular grid mesh. Normally, L3 has a coarser temporal and spatial resolution than L2.

2.2 The Radiative Transfer Equation

Let us consider the hypothesis of a non-scattering atmosphere, in which the only active processes are absorption and emission, and assume that atmospheric gases are in local thermodynamic equilibrium conditions (LTE). Then, the total radiance observed by a sensor located at the top of the atmosphere is the result of different physical processes, which can be summarised in three contributions: **upwelling radiance**, **downwelling radiance**, and **radiance contribution coming from the extra-terrestrial solar source** [130, 141]. All quantities depend on the wavenumber σ (cm^{-1}); the dependence over the directional angle is implicit.

The **upwelling radiance** $R^\uparrow(\sigma)$ in a fixed wavenumber σ (cm^{-1}) is given by the direct emission from the surface $R_s(\sigma)$ and atmosphere $R_a(\sigma)$. The surface radiance $R_s(\sigma)$ is the radiance directly emitted by the surface that travels through the atmosphere with a transmittance $\tau_0(\sigma)$ and an angle θ_{sat} with respect to the vertical spatial coordinate z (see Figure 2.3).

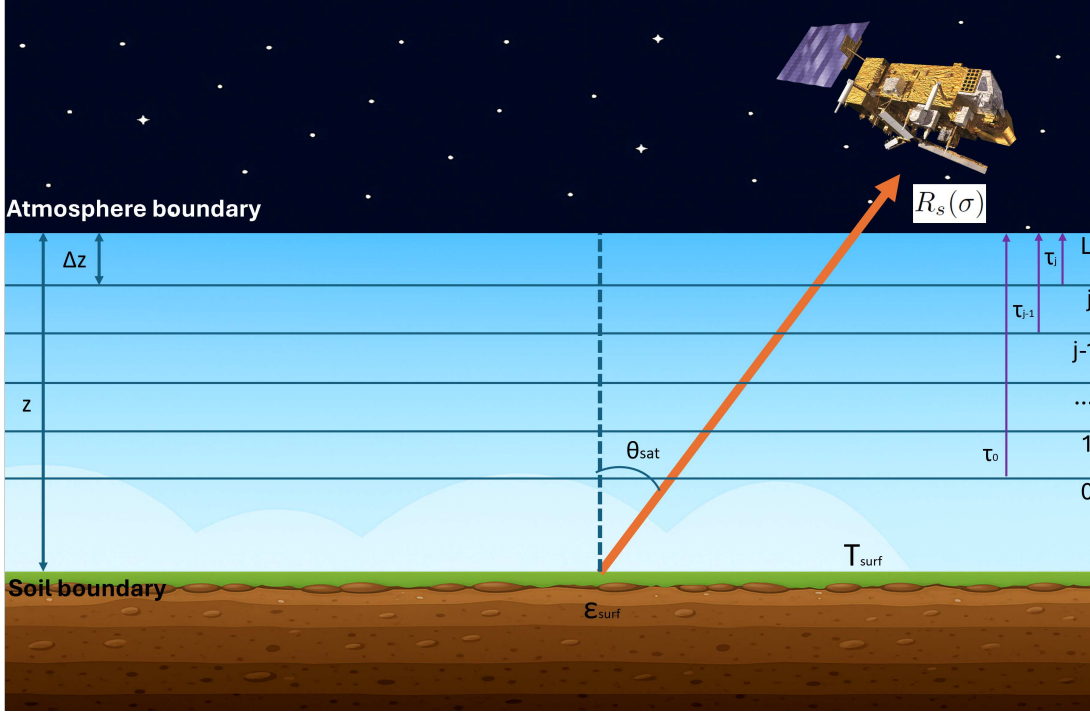


Figure 2.3: Schematic of the surface radiance $R_s(\sigma)$. Radiation emitted by the surface travels through the atmosphere at an angle θ_{sat} and transmittance $\tau_0(\sigma)$.

It can be expressed as:

$$R_s(\sigma) = \varepsilon_{surf}(\sigma)B(T_{surf}, \sigma)\tau_0(\sigma), \quad (2.1)$$

with

$\tau_0(\sigma)$ the total atmospheric transmittance from the surface to the top of the atmosphere,

$\varepsilon_{surf}(\sigma)$ the surface emissivity,

T_{surf} the skin temperature,

$B(T, \sigma) = \frac{c_1 \sigma^3}{\exp(c_2 \sigma / T) - 1}$ the Planck blackbody source term, where

$$c_1 = 1.1911 \times 10^{-8} \text{ W m}^{-2} \text{ sr}^{-1} (\text{cm}^{-1})^{-4} \text{ and}$$

$$c_2 = 1.4388 \text{ K (cm}^{-1})^{-1}.$$

The atmospheric component $R_a(\sigma)$ is the radiance directly emitted by the atmosphere along the slant path that travels through the atmosphere with an angle θ with respect to the vertical spatial coordinate z (see Figure 2.4). It is expressed as:

$$R_a(\sigma) = \int_0^{+\infty} B(T(z), \sigma) \frac{\partial \tau(\sigma)}{\partial z} dz, \quad (2.2)$$

where $\tau(\sigma)$ is the transmittance along $ds = dz/\mu$ $\mu = \cos(\theta)$ (with θ the satellite zenith angle) from altitude z to $+\infty$. Combining Eq. (2.1) and (2.2) we have the **upwelling radiance**:

$$R^\uparrow(\sigma) = R_s(\sigma) + R_a(\sigma) = \varepsilon_{surf}(\sigma)B(T_{surf}, \sigma)\tau_0(\sigma) + \int_0^{+\infty} B(T(z), \sigma) \frac{\partial \tau(\sigma)}{\partial z} dz. \quad (2.3)$$

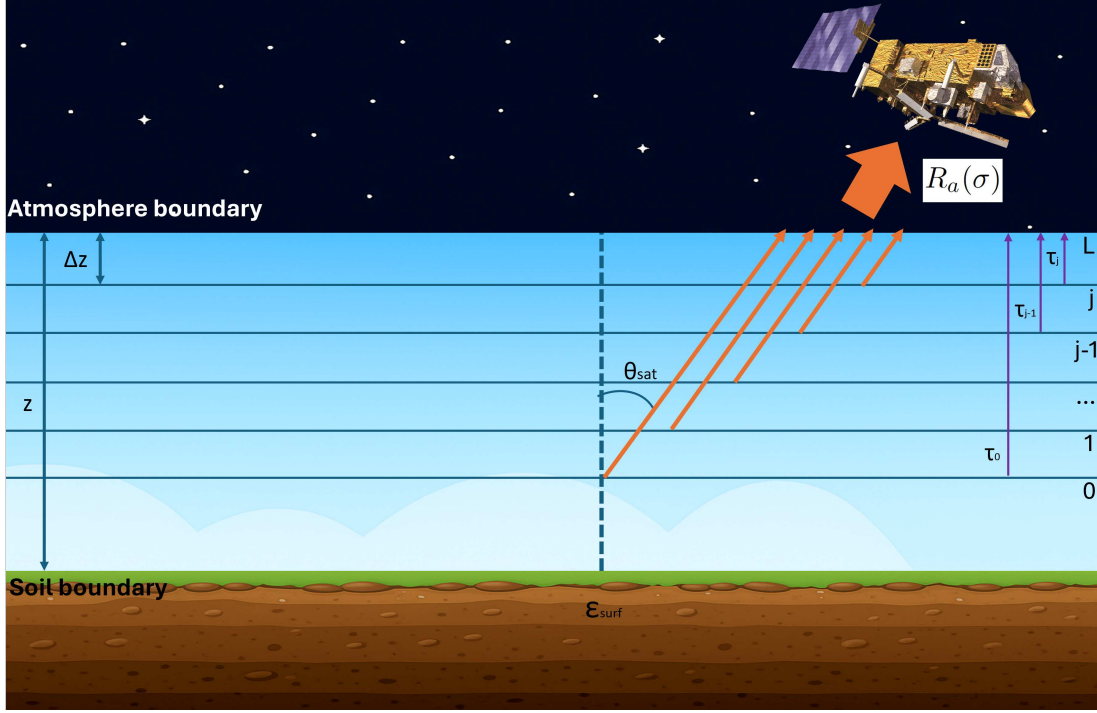


Figure 2.4: Schematic of the atmospheric component $R_a(\sigma)$, which is the radiation emitted by the atmosphere along the slant path travelling through the atmosphere at an angle θ_{sat} .

However, the atmosphere emits energy in all directions, not only in the observing one. For this reason another component to be considered is the **downwelling radiance** $R^\downarrow(\sigma)$, that is the radiance emitted by the atmosphere, which travels through it, reaches the surface, and is then reflected back to the observing sensor (see Figure 2.5).

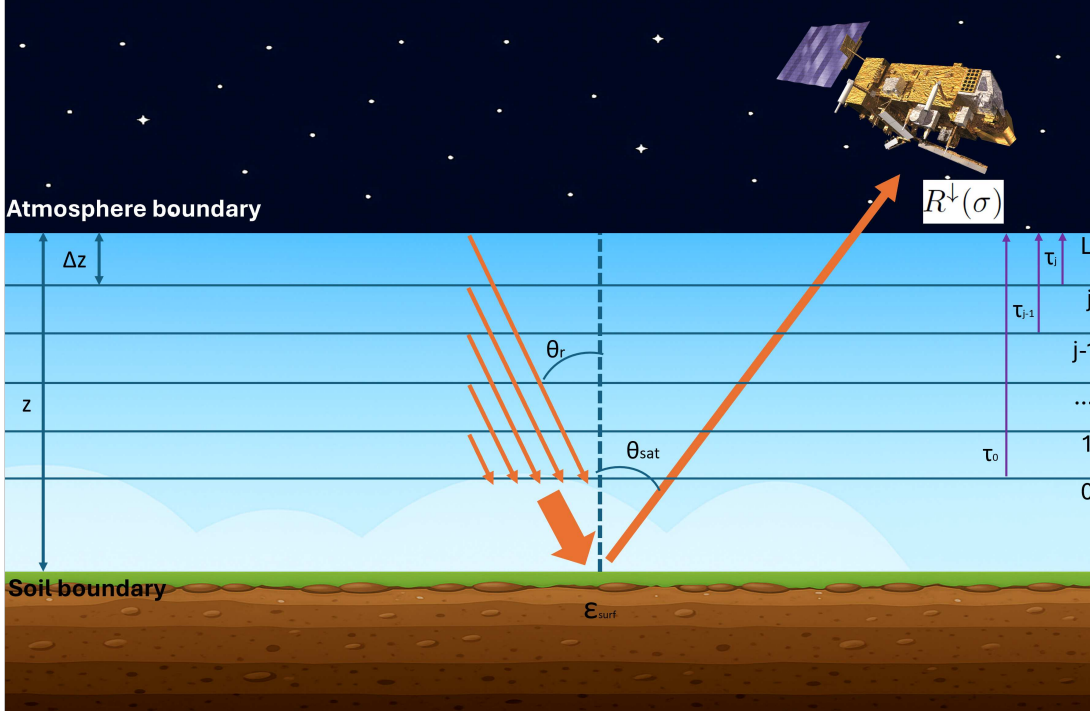


Figure 2.5: Schematic of the downwelling radiance $R^\downarrow(\sigma)$. Radiation emitted by the atmosphere travels through it reaching the surface at an angle θ_r , and then is reflected back to the observing sensor at an angle θ_{sat} .

The term $R^\downarrow(\sigma)$ is treated differently depending on the surface type. For the sea surface, a specular model was considered, see [95].

$$R^\downarrow(\sigma) = (\varepsilon_{surf}(\sigma) - 1)\tau_0^2(\sigma) \int_0^{+\infty} B(T(z), \sigma) \frac{\partial}{\partial z} \left(\frac{1}{\tau(\sigma)} \right) dz. \quad (2.4)$$

It should be noted that this term is of second order with respect to the upwelling one, because of the presence of $\tau_0^2(\sigma)$ in front of the integral along the slant path. Moreover, the ground emissivity $\varepsilon_{surf}(\sigma)$, in most practical applications in the infrared band, is greater than 0.9 and consequently this term is at most ten times smaller than the upwelling one. For land, a Lambertian (diffuse) model was considered:

$$R^\downarrow(\sigma) = (\varepsilon_{surf}(\sigma) - 1)\tau_0(\sigma) \int_0^{+\infty} B(T(z), \sigma) \frac{\partial \tau_*^f(\sigma)}{\partial z} dz, \quad (2.5)$$

where $\tau_*^f(\sigma) = 2 \int_0^1 \tau_*(\mu, z) \mu d\mu$ and τ_* is the transmittance from altitude z to $z = 0$ along the slant path in the direction $\mu = \cos(\theta)$ (with θ the satellite zenith angle). It is important to stress that the top-to-bottom transmittance τ_* should not be confused with the bottom-to-top transmittance τ . According to W.M. Elsasser [54] it is postulated that

$$\tau_*^f = \tau_*(\bar{\mu}, z), \quad (2.6)$$

i.e., the diffuse transmittance can be calculated as the transmittance function at a suitable cosine angle, the term $\frac{1}{\mu}$ is referred to as the diffusivity factor, and for practical calculations, the value $\frac{1}{\mu} = 1.66$ (corresponding to an effective zenith angle of 52.96°) yields accurate results, which depend on the optical depth; the effective zenith angle is spectrally dependent. For optical depth below 1, exact and approximate (through Eq. (2.6)) calculations nearly coincide.

The last piece to be added to obtain a first complete form of the radiative transfer equation is the **radiance contribution coming from the extra-terrestrial solar source**, when present. This is the solar radiation that travels through the atmosphere at an angle θ_{sun} with respect to the vertical, is reflected back by the surface, and reaches the observer along the direction θ_{sat} (see Figure 2.6).

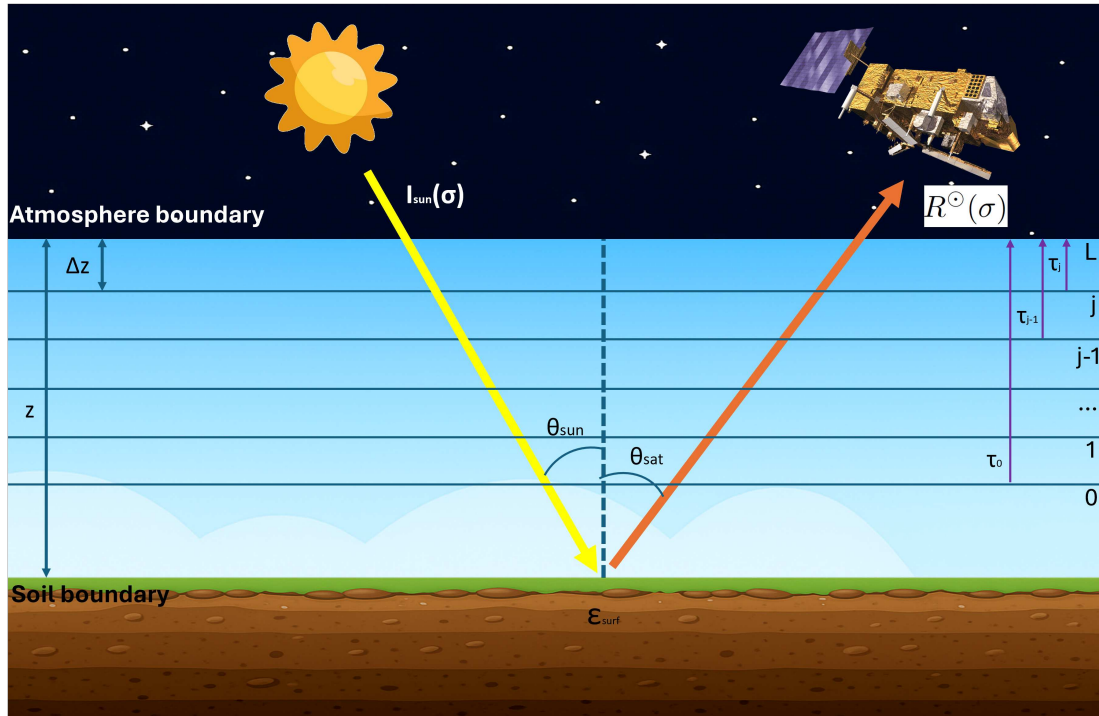


Figure 2.6: Schematic of the solar contribution $R^{\odot}(\sigma)$. Solar radiation travels through the atmosphere at an angle θ_{sun} , is reflected back by the surface, and reaches the observer along the direction θ_{sat} .

For water bodies, we have

$$R^{\odot}(\sigma) = r(\theta_{sun}, \theta_{sat}, \nu^2, \Phi) \tau_0(\theta_{sun}) \tau_0(\theta_{sat}) I_{sun}(\sigma), \quad (2.7)$$

where

$r(\theta_{\text{sun}}, \theta_{\text{sat}}, \nu^2, \Phi)$	is the bidirectional reflectance distribution function (BRDF) according to the Cox–Munk model [111], where ν^2 is a wind-speed parameter and $\Phi = \Phi_{\text{sat}} - \Phi_{\text{sun}}$ is the difference between satellite and solar azimuth angles,
$\tau_0(\theta_{\text{sun}})$	is the total atmospheric transmittance along the downwelling θ_{sun} -direction,
$\tau_0(\theta_{\text{sat}})$	is the total atmospheric transmittance along the upwelling θ_{sat} -direction,
$I_{\text{sun}}(\sigma)$	is the solar spectrum [33] incident on a normal surface and normalized to the solar disk solid angle as seen from Earth (6.8×10^{-5} sr), $[\text{W m}^{-2} (\text{cm}^{-1})^{-1}]$.

In the case of a Lambertian diffuser, i.e. over land, we have

$$R^{\odot}(\sigma) = \frac{1 - \varepsilon_{\text{surf}}(\sigma)}{\pi} \mu_{\text{sun}} \tau_0(\theta_{\text{sun}}) \tau_0(\theta_{\text{sat}}) I_{\text{sun}}(\sigma), \quad (2.8)$$

where $\mu_{\text{sun}} = \cos \theta_{\text{sun}}$.

In conclusion, we obtain the final form for the radiative transfer equation, in which the observed radiance is expressed as the sum of the terms (2.3), (2.4), (2.7) for water bodies:

$$\begin{aligned} R(\sigma) = R^{\text{surf}}(\sigma) + R^{\uparrow}(\sigma) + R^{\downarrow}(\sigma) + R^{\odot}(\sigma) = & \varepsilon_{\text{surf}}(\sigma) B(T_{\text{surf}}, \sigma) \tau_0(\sigma) + \int_0^{+\infty} B(T(z), \sigma) \frac{\partial \tau(\sigma)}{\partial z} dz + \\ & + (\varepsilon_{\text{surf}}(\sigma) - 1) \tau_0^2(\sigma) \int_0^{+\infty} B(T(z), \sigma) \frac{\partial}{\partial z} \left(\frac{1}{\tau(\sigma)} \right) dz + r(\theta_{\text{sun}}, \theta_{\text{sat}}, \nu^2, \Phi) \tau_0(\theta_{\text{sun}}) \tau_0(\theta_{\text{sat}}) I_{\text{sun}}(\sigma), \end{aligned} \quad (2.9)$$

and as the sum of the terms (2.3), (2.5), (2.8) for land:

$$\begin{aligned} R(\sigma) = R^{\text{surf}}(\sigma) + R^{\uparrow}(\sigma) + R^{\downarrow}(\sigma) + R^{\odot}(\sigma) = & \varepsilon_{\text{surf}}(\sigma) B(T_{\text{surf}}, \sigma) \tau_0(\sigma) + \int_0^{+\infty} B(T(z), \sigma) \frac{\partial \tau(\sigma)}{\partial z} dz + \\ & + (\varepsilon_{\text{surf}}(\sigma) - 1) \tau_0(\sigma) \int_0^{+\infty} B(T(z), \sigma) \frac{\partial \tau_*^f(\sigma)}{\partial z} dz + \frac{1 - \varepsilon_{\text{surf}}(\sigma)}{\pi} \mu_{\text{sun}} \tau_0(\theta_{\text{sun}}) \tau_0(\theta_{\text{sat}}) I_{\text{sun}}(\sigma). \end{aligned} \quad (2.10)$$

The radiative transfer equations (2.9) and (2.10) are rigorously correct only in the infrared region, because they neglect scattering effects; on the contrary, they are no longer correct in the visible region. Anyway, it should be pointed out that the solar radiation adds a significant contribution to the total radiance only for wavenumbers greater than $\approx 2000/\text{cm}$. Furthermore, these equations apply only to the clear-sky case, since the case of a non-scattering atmosphere is a good approximation for a clear sky.

Eqs. (2.9) – (2.10) require further manipulation steps because they cannot be directly implemented in a model that can be solved. The key passage is represented by its **discretization**. This in turn implies that the atmosphere is described with an arbitrary degree of approximation: instead of considering the temperature and gases/particle concentrations as a continuum, the atmosphere is divided in a certain (arbitrary) number N_L of discrete layers (see Figure 2.7). In principle, the greater the number of layers, the more accurately the atmosphere is described. Each layer is assumed to be characterized by a certain, homogeneous temperature, pressure and composition.

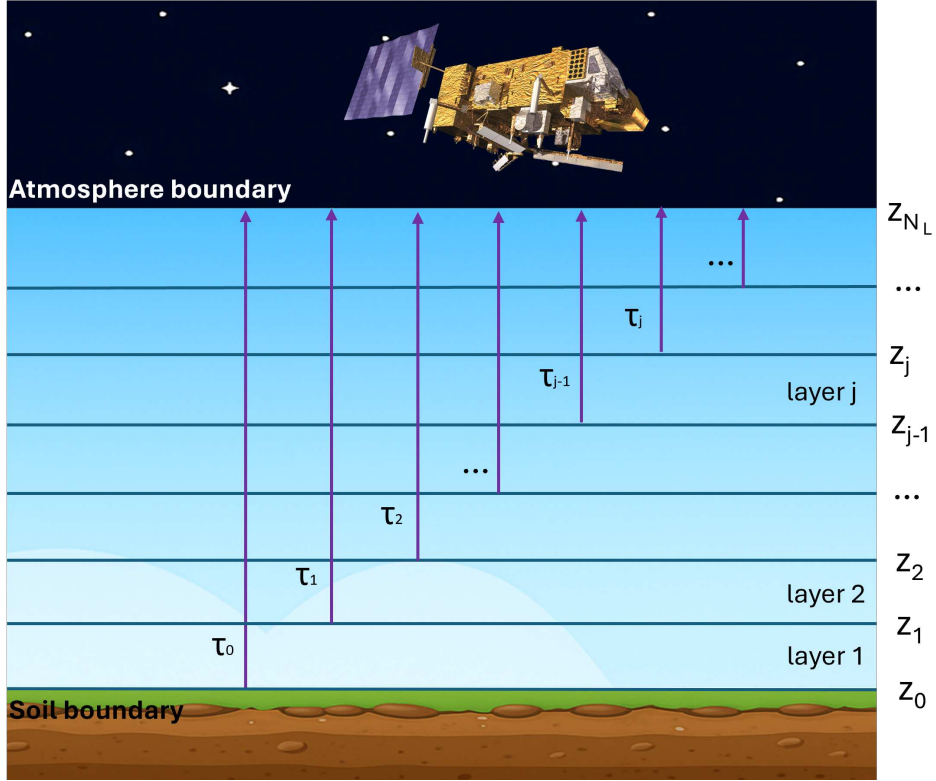


Figure 2.7: Layering scheme of the atmosphere, with layers numbered from 0 to N_L and their corresponding transmittances.

With this hypothesis, each integral in Eq. (2.9) - (2.10) becomes a sum over the layers. The discretized version of Eq. (2.9) assumes the following expression:

$$\begin{aligned}
 R(\sigma) = & \varepsilon_{surf} B(T_{surf}) \tau_0 + \sum_{j=1}^{N_L} B(T_j) (\tau_j - \tau_{j-1}) + (\varepsilon_{surf} - 1) \tau_0^2 \sum_{j=1}^{N_L} B(T_j) (\tau_j^{-1} - \tau_{j-1}^{-1}) + \\
 & + r(\theta_{sun}, \theta_{sat}, \nu^2, \Phi) \tau_0(\theta_{sun}) \tau_0(\theta_{sat}) I_{sun},
 \end{aligned} \tag{2.11}$$

while for land Eq. (2.10) becomes:

$$R(\sigma) = \varepsilon_{surf} B(T_{surf}) \tau_0 + \sum_{j=1}^{N_L} B(T_j) (\tau_j - \tau_{j-1}) + (\varepsilon_{surf} - 1) \tau_0 \sum_{j=1}^{N_L} B(T_j) (\tau_*(\bar{\mu})_j - \tau_*(\bar{\mu})_{j-1}) + \frac{1 - \varepsilon_{surf}}{\pi} \mu_{sun} \tau_0 (\theta_{sun}) \tau_0 (\theta_{sat}) I_{sun}. \quad (2.12)$$

Note that the dependence on the wavenumber σ is not made explicit for brevity. Here τ_j is the total transmittance from the top of the j -th layer to ∞ , and τ_{j-1} is the total transmittance from the bottom of the j -th layer to ∞ , with $\tau_{N_L} = 1$. In addition, T_j is the average temperature of the j -th layer. In this way, each layer is assumed to emit radiation at its characteristic temperature i.e., a layer-equivalent temperature. The same scheme is followed to calculate, layer by layer, the values of air density and gas concentrations. It is possible to write explicitly the expression for the transmittance τ_j in the cases of clear sky:

$$\tau_j = \prod_{i=j+1}^{N_L} \exp[-(\chi_{gas,i} + \chi_{aer,i})], \quad (2.13)$$

where $\chi_{C,i}$ is the total single-layer optical depth in the absence of clouds, and $\chi_{aer,i}$ is the optical depth of aerosol particles in the i -th layer. Again, the dependence on wavenumber is not made explicit. In the clear sky case, the transmittance is calculated considering both gases and aerosols optical depths.

Equations (2.9), (2.10) and (2.13) are the basis to implement radiative transfer into a consistent model. Apart from surface input parameters, the solution of the radiative transfer equation deals with the problem of quantifying, for each layer, the atmospheric transmittance in the whole spectral range of interest, which depends on the layer optical depth. At each wavenumber, the optical depth varies according to the spectral properties of gases, aerosols and clouds, and to the layer temperature.

2.3 The Inversion of the Radiative Transfer Equation

To estimate the thermodynamic state of the atmosphere, the radiative transfer equations (2.11) and (2.12) must be inverted. The retrieval module δ -IASI implements an iterative algorithm for the **optimal estimation** of the thermodynamic state of the atmosphere. The retrieval algorithm follows Rodgers optimal estimation method [197] by considering an iterative Gauss–Newton scheme. In detail, let us indicate with $\mathbf{R}_{obs} = (R(\sigma_1), \dots, R(\sigma_N))^T \in \mathbb{R}^{N \times 1}$ the vector of observed radiances, with $\mathbf{v} = (v_1, \dots, v_m)^T \in \mathbb{R}^{m \times 1}$ the vector of geophysical parameters (atmospheric and surface), $N > M$, then we can express Eq. (2.11) and (2.12) in compact form as

$$\mathbf{R}_{obs} = F(\mathbf{v}) + \varepsilon \quad (2.14)$$

where ε is the additive noise accounting for observational, i.e. instrumental detector noise ε_r , and forward model bias ε_m . We assume that the model noise ε_m can be neglected with respect to

the random error ε_r , that we assume Gaussian with $\mathbf{0}$ mean and covariance $\mathbf{S}_\varepsilon$ (the subscript r was omitted to simplify notation).

The problem of solving for $\mathbf{v}$ from Eq. (2.14) is ill-posed, see [197], because there are many atmospheric and surface states $\mathbf{v}$ that can explain the same measurement $\mathbf{R}_{obs}$. To solve this ill-posed problem, the usual way is to define a cost function that combines the information provided by the measurement with *a priori* known characteristics of the atmospheric state to determine the best solution from all the possible ones, which are consistent with the observations.

Assuming Gaussian *a priori* information about the state parameter $\mathbf{v}$, independent of the instrumental one, i.e.,

$$p(\mathbf{v}) \sim N\left(\mathbf{v}_a, \frac{1}{\gamma} \mathbf{S}_a\right), \quad (2.15)$$

where $\gamma \in (0, +\infty)$ quantifies how strongly we believe that $\mathbf{v}$ should be close to $\mathbf{v}_a$. The predictive distribution $[v|\mathbf{R}_{obs}]$ is no longer Gaussian because of the nonlinearity of F

$$-2 \ln P(\mathbf{v}|\mathbf{R}_{obs}) = (\mathbf{R}_{obs} - F(\mathbf{v}))^T \mathbf{S}_\varepsilon^{-1} (\mathbf{R}_{obs} - F(\mathbf{v})) + \gamma (\mathbf{v} - \mathbf{v}_a)^T \mathbf{S}_a^{-1} (\mathbf{v} - \mathbf{v}_a). \quad (2.16)$$

Note that the term due to the *a priori* information, $\gamma (\mathbf{v} - \mathbf{v}_a)^T \mathbf{S}_a^{-1} (\mathbf{v} - \mathbf{v}_a)$ can equivalently be interpreted as a regularization term used to solve an ill-posed problem, controlled by the regularization parameter γ . The maximum probability state $\hat{\mathbf{v}}$ is the solution to the minimization problem

$$\underset{\mathbf{v}}{\operatorname{argmin}} (\mathbf{R}_{obs} - F(\mathbf{v}))^T \mathbf{S}_\varepsilon^{-1} (\mathbf{R}_{obs} - F(\mathbf{v})) + \gamma (\mathbf{v} - \mathbf{v}_a)^T \mathbf{S}_a^{-1} (\mathbf{v} - \mathbf{v}_a), \quad (2.17)$$

and this is equivalent to solving the following non linear equation

$$g(\mathbf{v}) = -\mathbf{K}^T(\mathbf{v}) \mathbf{S}_\varepsilon^{-1} (\mathbf{R}_{obs} - F(\mathbf{v})) + \gamma \mathbf{S}_a^{-1} (\mathbf{v} - \mathbf{v}_a) = 0,$$

where $\mathbf{K}(\mathbf{v}) = \nabla_{\mathbf{v}} F(\mathbf{v})$ is the Jacobian matrix of order $N \times m$. Considering the classical Newton iteration scheme we obtain

$$\mathbf{v}_{\ell+1} = \mathbf{v}_\ell - (\nabla_{\mathbf{v}} g(\mathbf{v}_\ell))^{-1} g(\mathbf{v}_\ell)$$

which requires the evaluation of the Hessian of $F(\mathbf{v})$

$$\nabla_{\mathbf{v}} g(\mathbf{v}) = \gamma \mathbf{S}_a^{-1} + \mathbf{K}^T \mathbf{S}_\varepsilon^{-1} \mathbf{K} - (\nabla_{\mathbf{v}} \mathbf{K}^T) \mathbf{S}_\varepsilon^{-1} (\mathbf{R}_{obs} - F(\mathbf{v})).$$

By dropping the second derivative term, $\nabla_{\mathbf{v}} g(\mathbf{v}) \approx \gamma \mathbf{S}_a^{-1} + \mathbf{K}^T \mathbf{S}_\varepsilon^{-1} \mathbf{K}$ and the procedure relaxes to the Gauss-Newton iteration scheme

$$\mathbf{v}_{\ell+1} = \mathbf{v}_\ell + (\gamma \mathbf{S}_a^{-1} + \mathbf{K}_\ell^T \mathbf{S}_\varepsilon^{-1} \mathbf{K}_\ell)^{-1} [\mathbf{K}_\ell^T \mathbf{S}_\varepsilon^{-1} (\mathbf{R}_{obs} - F(\mathbf{v}_\ell)) - \gamma \mathbf{S}_a^{-1} (\mathbf{v}_\ell - \mathbf{v}_a)]. \quad (2.18)$$

By expressing $\mathbf{v}_{\ell+1}$ as a departure from the prior mean $\mathbf{v}_a$ rather than $\mathbf{v}_\ell$, Eq. (2.18) can be

rearranged as

$$\mathbf{v}_{\ell+1} = \mathbf{v}_a + \left(\gamma_\ell \mathbf{S}_a^{-1} + \mathbf{K}_\ell^T \mathbf{S}_\varepsilon^{-1} \mathbf{K}_\ell \right)^{-1} \mathbf{K}_\ell^T \mathbf{S}_\varepsilon^{-1} \left[(\mathbf{R}_{obs} - F(\mathbf{v}_\ell)) + \mathbf{K}_\ell (\mathbf{v}_\ell - \mathbf{v}_a) \right], \quad (2.19)$$

and a typical choice is $\mathbf{v}_a$ for the starting value $\mathbf{v}_0$ for $\ell = 0$ (*first guess*) in the iteration. Moreover, the regularization parameter γ depends on the iteration ℓ and must be optimized at each iteration according to some criterion; in the particular case $\gamma = 1$ in Eq. (2.15), the technique coincides with the optimal estimation discussed in [197].

Note that $\mathbf{v}_{\ell+1}$ in Eq. (2.19) is the solution of the following minimization problem

$$\min_{\mathbf{v}} \left\| \mathbf{S}_\varepsilon^{-1/2} \mathbf{K}_\ell (\mathbf{v} - \mathbf{v}_a) - \mathbf{S}_\varepsilon^{-1/2} [(\mathbf{R}_{obs} - F(\mathbf{v}_\ell)) + \mathbf{K}_\ell (\mathbf{v}_\ell - \mathbf{v}_a)] \right\|_2^2 + \gamma_\ell \left\| \mathbf{S}_a^{-1/2} (\mathbf{v} - \mathbf{v}_a) \right\|_2^2 \quad (2.20)$$

The covariance matrix $\hat{\mathbf{S}} = \mathbb{E}[(\mathbf{v} - \hat{\mathbf{v}})(\mathbf{v} - \hat{\mathbf{v}})]$ of the solution $\hat{\mathbf{v}}$ in the limiting case $\ell \rightarrow \infty$ will be

$$\hat{\mathbf{S}} = \left(\hat{\gamma} \mathbf{S}_a^{-1} + \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \hat{\mathbf{K}} \right)^{-1} \left(\hat{\gamma}^2 \mathbf{S}_a^{-1} + \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \hat{\mathbf{K}} \right) \left(\hat{\gamma} \mathbf{S}_a^{-1} + \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \hat{\mathbf{K}} \right)^{-1} \quad (2.21)$$

with $\hat{\mathbf{K}} = \nabla_{\mathbf{v}} F(\mathbf{v})|_{\mathbf{v}=\hat{\mathbf{v}}}$ jacobian evaluated in the solution $\hat{\mathbf{v}}$ and $\hat{\gamma}$ optimal regularization parameter corresponding to $\hat{\mathbf{v}}$ chosen by some ad-hoc criterion.

Eq. (2.19) is the solution of the linearized form of Eq. (2.17) and, as any penalty method, is a biased estimate of the true state of the atmosphere, i.e.

$$\boldsymbol{\delta} = \mathbb{E}(\hat{\mathbf{v}}) - \mathbf{v} \neq 0.$$

The bias $\boldsymbol{\delta}$ can be easily estimated. First of all, in Eq. (2.14) let us consider the first order Taylor expansion around $\hat{\mathbf{v}}$

$$\mathbf{R}_{obs} = F(\mathbf{v}) + \boldsymbol{\varepsilon} \approx F(\hat{\mathbf{v}}) + \mathbf{K}(\mathbf{v} - \hat{\mathbf{v}}) + \boldsymbol{\varepsilon}, \quad (2.22)$$

then, in the limiting case $\ell \rightarrow \infty$ and $\mathbf{v}_\ell \rightarrow \hat{\mathbf{v}}$ and using Eq. (2.22), Eq. (2.19) becomes

$$\begin{aligned} \hat{\mathbf{v}} &= \mathbf{v}_a + \left(\hat{\gamma} \mathbf{S}_a^{-1} + \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \hat{\mathbf{K}} \right)^{-1} \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \left[(\mathbf{R}_{obs} - F(\hat{\mathbf{v}})) + \hat{\mathbf{K}} (\hat{\mathbf{v}} - \mathbf{v}_a) \right] \\ &= \mathbf{v}_a + \left(\hat{\gamma} \mathbf{S}_a^{-1} + \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \hat{\mathbf{K}} \right)^{-1} \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \left[\hat{\mathbf{K}} (\mathbf{v} - \mathbf{v}_a) + \boldsymbol{\varepsilon} \right]. \end{aligned} \quad (2.23)$$

Since the noise $\boldsymbol{\varepsilon}$ has zero mean, it follows

$$\begin{aligned} \boldsymbol{\delta} &= \mathbb{E}(\hat{\mathbf{v}}) - \mathbf{v} = \mathbf{v}_a + \left(\hat{\gamma} \mathbf{S}_a^{-1} + \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \hat{\mathbf{K}} \right)^{-1} \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \left[\hat{\mathbf{K}} (\mathbf{v} - \mathbf{v}_a) \right] - \mathbf{v} \\ &= \left(\hat{\mathbf{A}} - \mathbf{I}_m \right) (\mathbf{v} - \mathbf{v}_a), \end{aligned} \quad (2.24)$$

where $\hat{\mathbf{A}} = \left(\hat{\gamma} \mathbf{S}_a^{-1} + \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \hat{\mathbf{K}} \right)^{-1} \hat{\mathbf{K}}^T \mathbf{S}_\varepsilon^{-1} \hat{\mathbf{K}}$ is the *Averaging Kernel* matrix. From this last

equation, we easily derive

$$\begin{aligned}\frac{\partial \delta}{\partial \mathbf{v}} &= (\hat{\mathbf{A}} - \mathbf{I}_m) \\ \frac{\partial \hat{\mathbf{v}}}{\partial \mathbf{v}} &= \hat{\mathbf{A}}.\end{aligned}\tag{2.25}$$

The *Averaging Kernel* matrix was introduced by [10]; it is also known as the *model-resolution* matrix [162], the *state resolution* matrix or the *resolving kernel* and plays a fundamental role in the assessment of the retrieved information content because it describes the subspace where the retrieval must lie.

It is a common practice to use the above derivative matrix as a measure of the spatial vertical resolution of the retrieval. Each row of $\hat{\mathbf{A}}$ defines the averaging kernel for one particular layer in the retrieved profile $\hat{\mathbf{v}}$. Each element in that row represents the relative weight of the “true” value at each layer to the retrieved value and Eq. (2.25) gives how the bias propagates from the nearby layers or grid points to a given layer.

The use of averaging kernels as a quantitative definition of spatial resolution is not immune to criticism since it addresses only one side of the problem, that is the bias, whereas it completely ignores the covariance of the retrieval, Eq. (2.21). Indeed, if $\hat{\gamma} = 0$ we have that the averaging kernel is the identity matrix. This simply expresses the well-known unbiasedness property of unconstrained least squares, [122]. If we interpret this result in terms of spatial resolution, then the effective resolving kernels would be Dirac functions coinciding with the pressure or altitude grid used for representing the state vector, $\mathbf{v}$, and we would have achieved the highest spatial resolution with the given data. However, this conclusion, which may be read in many averaging kernel papers, is inconsistent since the covariance matrix has, in general, non-null off-diagonal elements even for $\hat{\gamma} = 0$. The retrieval is, hence, correlated and the state vector has not been independently resolved by the data set.

2.3.1 Stopping Criterion

The convergence of the Newton method is of second order, and Gauss-Newton is of first order, but if the neglected term, the Hessian, is small, i.e. the problem is less than grossly nonlinear, Gauss-Newton will converge quickly and as the minimum is approached the ignored term becomes smaller and convergence approaches second order. Since the procedure used to determine the optimal solution is iterative, a stopping criterion is required. A commonly used test is to look directly at the χ^2 distribution. Indeed, since $(\mathbf{R}_{obs} - F(\mathbf{v}))^T \mathbf{S}_\epsilon^{-1} (\mathbf{R}_{obs} - F(\mathbf{v})) \sim \chi_N^2$ with N degrees of freedom, the iterative process can be stopped when the computed value of χ^2 at iteration ℓ , i.e. $\chi_\ell^2 = (\mathbf{R}_{obs} - F(\mathbf{v}_\ell))^T \mathbf{S}_\epsilon^{-1} (\mathbf{R}_{obs} - F(\mathbf{v}_\ell))$ is below the threshold χ_α^2 , where χ_α^2 is the value of a χ^2 variable with N degree of freedom at the confidence interval $1 - \alpha$. However, this test alone is inadequate and may not be satisfied because of unknown systematic effects which are likely to affect the forward model. For this reason, the following three-level constraint is generally implemented according to an IF structure with an OR logic:

- $\chi_\ell^2 \leq \chi_\alpha^2$,

- $\frac{\chi_\ell^2 - \chi_{\ell-1}^2}{\chi_{\ell-1}^2} \leq 0.1$
- $\chi_\ell^2 \geq \chi_{\ell-1}^2$

The first two constraints are standard for iterative methods with normal runs, on the contrary, when the cycle stops because of the third constraint, it is likely that the iterative Newtonian mechanism just fails.

2.3.2 Efficient Computation

Considering Eq. (2.19) and indicating with

$$\begin{aligned}\mathbf{x}_{\ell+1} &= \mathbf{v}_{\ell+1} - \mathbf{v}_a \\ \mathbf{z}_\ell &= \mathbf{S}_\varepsilon^{-1/2} [(\mathbf{R}_{obs} - F(\mathbf{v}_\ell)) + \mathbf{K}_\ell (\mathbf{v}_\ell - \mathbf{v}_a)] \\ \mathbf{J}_\ell &= \mathbf{S}_\varepsilon^{-1/2} \mathbf{K}_\ell\end{aligned}$$

then

$$\left(\gamma_\ell \mathbf{S}_a^{-1/2} \mathbf{S}_a^{-1/2} + \mathbf{J}_\ell^T \mathbf{J}_\ell \right) \mathbf{x}_{\ell+1} = \mathbf{J}_\ell^T \mathbf{z}_\ell. \quad (2.26)$$

Defining $\mathbf{G}_\ell = \mathbf{J}_\ell \mathbf{S}_a^{1/2}$ and $\mathbf{u}_{\ell+1} = \mathbf{S}_a^{-1/2} \mathbf{x}_{\ell+1}$, then Eq. (2.26) assumes the form of a *ridge regression*

$$(\gamma_\ell \mathbf{I}_m + \mathbf{G}_\ell^T \mathbf{G}_\ell) \mathbf{u}_{\ell+1} = \mathbf{G}_\ell^T \mathbf{z}_\ell. \quad (2.27)$$

Considering now the Singular Value Decomposition (SVD) of matrix $\mathbf{G}_\ell = \mathbf{U}_\ell \mathbf{D}_\ell \mathbf{V}_\ell^T$, with $\mathbf{U}_\ell \in \mathbb{R}^{N \times m}$, $\mathbf{D}_\ell = \text{diag}(\sigma_{1,\ell}, \dots, \sigma_{m,\ell}) \in \mathbb{R}^{m \times m}$, and $\mathbf{V}_\ell \in \mathbb{R}^{m \times m}$, then Eq. (2.27) can be rewritten as

$$\mathbf{u}_{\ell+1} = \mathbf{V}_\ell (\gamma_\ell \mathbf{I}_m + \mathbf{D}_\ell^2)^{-1} \mathbf{D}_\ell \mathbf{U}_\ell^T \mathbf{z}_\ell. \quad (2.28)$$

Note that in Eq. (2.28) the evaluation over a grid of γ_ℓ values requires just the update of the kernel $(\gamma_\ell \mathbf{I}_m + \mathbf{D}_\ell^2)^{-1}$ that is a diagonal matrix, so it's $O(m)$.

2.3.3 Choice of the Regularization Parameter γ

For the optimal choice of the regularization parameter a well-known criterion is the *L-curve* [87]. It is based on the study of the curve, called *L-curve* because of its shape, obtained by plotting the L_2 norm of the regularization term $\left\| \mathbf{S}_a^{-1/2} \mathbf{x}_{\ell+1} \right\|_2$ against the L_2 norm of the residual $\left\| \mathbf{J}_\ell \mathbf{x}_{\ell+1} - \mathbf{z}_\ell \right\|_2$, see Eq. (2.26), as a function of $\gamma_\ell \in (0, +\infty)$. The optimal regularization parameter is then the value of γ_ℓ corresponding to the point of maximum curvature (i.e., the

sharpest corner) of the *L-curve*. The curvature is expressed as a function of γ_ℓ by

$$c(\gamma_\ell) = \frac{|\rho'(\gamma_\ell)\eta''(\gamma_\ell) - \rho''(\gamma_\ell)\eta'(\gamma_\ell)|}{\left[(\rho'(\gamma_\ell))^2 + (\eta'(\gamma_\ell))^2\right]^{3/2}}$$

where

$$\begin{aligned}\rho(\gamma_\ell) &= \|\mathbf{J}_\ell \mathbf{x}_{\ell+1} - \mathbf{z}_\ell\|_2 \\ \eta(\gamma_\ell) &= \left\| \mathbf{S}_a^{-1/2} \mathbf{x}_{\ell+1} \right\|_2,\end{aligned}$$

and can be easily evaluated by using SVD of matrix $\mathbf{G}_\ell$.

2.3.4 Choice of the First Guess

In general, the *first guess* $\mathbf{v}_0$ for the Gauss-Newton iteration scheme is chosen to be equal to the *a priori* mean $\mathbf{v}_a$. The *a priori* knowledge about the state of the atmosphere is from *climatology*, i.e. the mean and the covariance of an ensemble of states deriving from a predetermined database according to spatial and temporal colocalization with the measured radiance spectrum.

2.4 Retrieval of Geophysical Parameters on a Regular Grid

The retrieval of geophysical parameters from IASI radiances is limited by the nature of the sensor. Since IASI is a TIR sounder, it cannot penetrate thick cloud layers (clouds are opaque in the TIR), resulting in reliable retrievals only for clear-sky pixels. Cloud-contaminated pixels are dominated by cloud-top emission and carry little information on the surface or lower troposphere, requiring a filtering step to discard pixels with cloud fractions exceeding a given threshold (typically 10%). This introduces **missing data**, requiring an interpolation step to transform the sparsely populated, non-uniform L2 observations into evenly-gridded maps (L3).

Let us assume we want to retrieve the true model state of a geophysical variable $\mathcal{Y}$ at spatial locations $S = \{s_1, s_2, \dots, s_p\}$ that is observed only over a subset of spatial locations $n < p$, i.e., at $s_{(1)}, \dots, s_{(n)}$, where the notation $(j), j = 1, \dots, n$ indicates any point of S . Let us indicate with $\mathbf{y} \in \mathbb{R}^{n \times 1}$ the vector of observations. Suppose we have a set of features $\mathbf{x}_i \in \mathbb{R}^{d \times 1}, i = 1, \dots, p$, i.e., available for each spatial location in S . These features (e.g., longitude/latitude, day-of-year, land cover, ancillary meteorological fields, and others) are related somehow to our geophysical variable $\mathbf{y}$. From a mathematical point of view, we want to model the L2 spatial observation $y_i, i = 1, \dots, n$ as $y_i = \mu(\mathbf{x}_i) + \varepsilon_i$, where $\mu : \mathbb{R}^d \rightarrow \mathbb{R}$ is the unknown regression function to be estimated, $\mathbf{x} \in \mathbb{R}^d$ is the feature vector, and ε_i is the error term. If we know μ , we can take advantage of $\mathbf{x}$ and compute the true model state of $\mathcal{Y}$ over S .

Citing Mitchell (1997) [165]:

“Any hypothesis found to approximate the target function well over a sufficiently large set of training examples will also approximate the target function well over other unobserved examples.”

The selection of μ is very important: it establishes the model's inductive bias, controls the bias-variance trade-off, and determines how well the model generalizes. In this work, a number of Machine Learning (ML) algorithms with complementary strengths have been explored, including Random Forest (RF) [24], Gradient-Boosted Trees (GBT) [69], Neural Network (NN) [79], and Gaussian Process Regression (GPR) [193]. Then, these models were combined in an ensemble approach using Stacked Regression [23] to increase robustness and accuracy.

2.4.1 Tree-based Methods

RF and GBT are both **ensemble methods** that combine multiple decision trees, such as Decision Trees or Classification and Regression Trees (CART), to improve predictive performance.

- In **Random Forest (RF)**, M trees are created through bagging [24] and random feature selection. Each tree is independently trained on a randomly selected subset of the training data, with a series of splitting rules applied to build the tree. The essential idea in bagging is to average many noisy but approximately unbiased models and reduce the variance. Trees are ideal candidates for bagging, since they can capture complex interaction structures in the data, and if grown sufficiently deep, have relatively low bias. See [88] for more details. The bagging process can be summarized as follows:

1. For $m = 1, \dots, M$ (where M is the total number of trees):
 - (a) Sample, with replacement, k training examples from $\mathbf{x}, \mathbf{y}$; call these $\mathbf{x}_m, \mathbf{y}_m$.
 - (b) Train a classification or regression tree f_m on $\mathbf{x}_m, \mathbf{y}_m$ considering only a random subset of the features. This random feature selection enhances decorrelation between trees. Recursively repeat the following steps for each terminal node of the tree, until the minimum node size is reached.
 - i. Select p variables at random from the d variables.
 - ii. Pick the best variable/split-point among the p .
 - iii. Split the node into two daughter nodes.
2. After training, predictions for unseen samples $\mathbf{x}'$ are made by aggregating the predictions from all individual trees, and for regression tasks, the final prediction is obtained by averaging:

$$\hat{f}(\mathbf{x}') = \frac{1}{M} \sum_{m=1}^M f_m(\mathbf{x}').$$

By aggregating M decorrelated trees, RF effectively reduces variance and produces a robust final estimate.

- **Gradient-Boosted Trees (GBT)**, on the other hand, uses boosting [69] to aggregate trees. The key difference is that in bagging, each tree is built independently, while in boosting, each new tree is added sequentially, specifically designed to correct errors made by previous

trees. A generic GBT algorithm for regression, as described in [88], can be written as follows:

1. Initialize $f_0(x) = \arg \min_{\gamma} \sum_{i=1}^n L(y_i, \gamma)$ where L is the loss function.

2. For $m = 1$ to M :

(a) For $i = 1, \dots, n$, compute the pseudo residuals:

$$r_i^{(m)} = - \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f(\mathbf{x}_i)} \right]_{f=f_{m-1}}.$$

(b) Fit a regression tree to the targets $r_i^{(m)}$, giving terminal regions R_{jm} , $j = 1, \dots, J_m$.

(c) For $j = 1, \dots, J_m$ compute:

$$\gamma_{jm} = \arg \min_{\gamma} \sum_{\mathbf{x}_i \in R_{jm}} L(y_i, f_{m-1}(\mathbf{x}_i) + \gamma).$$

(d) Update:

$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \eta \sum_{j=1}^{J_m} \gamma_{jm} \mathbb{I}(\mathbf{x} \in R_{jm}),$$

where $\mathbb{I}(\cdot)$ is the indicator function and η is the learning rate.

3. Output $\hat{f}(\mathbf{x}) = f_M(\mathbf{x})$.

In this work, I used the least-squares loss function, simplifying the initialization to $f_0(x) = \bar{y}$, and the residuals to $r_i^{(m)} = y_i - f(\mathbf{x}_i)$.

This iterative approach enables GBT to focus on improving the predictions where prior models underperformed, often resulting in enhanced accuracy.

2.4.2 Gaussian Process

A **Gaussian Process (GP)** $g(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$ is a stochastic process fully specified by its mean function $m(\mathbf{x})$ and covariance function $k(\mathbf{x}, \mathbf{x}')$, consisting of an infinite collection of random variables, where any finite subset has a multivariate Gaussian distribution [193].

In realistic scenarios, it is often assumed the mean $m(\mathbf{x}) = \mathbf{h}(\mathbf{x})^t \boldsymbol{\beta}$, where $\mathbf{h}(\cdot)$ are a set of fixed basis functions that transform the original feature vector $\mathbf{x}$ in $\mathbb{R}^d$ into a new feature vector $\mathbf{h}(\mathbf{x})$ in $\mathbb{R}^p$, where parameters $\boldsymbol{\beta}$ must be inferred by data. Moreover, data are often noisy hence we typically have access only to noisy versions of true function values, $y_i = \mathbf{h}(\mathbf{x}_i)^t \boldsymbol{\beta} + f(\mathbf{x}_i) + \varepsilon_i$, $i = 1, \dots, n$, where $f(\mathbf{x}) \sim \mathcal{GP}(\mathbf{0}, k(\mathbf{x}, \mathbf{x}'))$ and $\varepsilon \sim \mathcal{N}(\mathbf{0}, \sigma_n^2 \mathbf{I})$ represents additive independent and identically distributed (i.i.d.) Gaussian noise with covariance $\sigma_n^2 \mathbf{I}$ [193]. This formulation expresses that the data is close to a global linear model with the residuals being modelled by a GP and the model fitting optimises over the parameters jointly with the hyperparameters of the covariance function.

The kernel $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$, $i, j = 1, \dots, n$ encodes the similarity between the input points according to some metric, i.e., points characterised by similar features must have similar target values y and thus, training points that are near to a test point should be informative about the prediction at that point. This is translated in terms of correlation. Indicating with $r = d(\mathbf{x}_i, \mathbf{x}_j)$ any distance between points i, j , the most common kernel function to account for such a similarity between points is the Squared Exponential (SE)

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{r}{2l^2}\right) \quad (2.29)$$

where l , also called the length scale parameter, indicates how quickly the correlation between two points drops as their distance increases. This kernel is infinitely differentiable, which means that the GP has mean square derivatives of all orders, and is thus very smooth and such strong smoothness assumptions can be unrealistic for modelling many physical processes. So an alternative option is the Matérn class defined as

$$k(\mathbf{x}_i, \mathbf{x}_j) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}r}{l}\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}r}{l}\right) \quad (2.30)$$

with $\nu > 0, l > 0$ and K_ν is a modified Bessel Function [1] (see section 9.6). Note that for $\nu \rightarrow \infty$ we obtain the SE covariance function. For the Matérn class, the process $f(\mathbf{x})$ is k -times Mean Square differentiable if and only if $\nu > k$. For the definition of Mean Square Differentiability, see Section 4.1.1 in [193]. When $\nu = p + 1/2$ with p a non-negative integer, the kernel becomes a product of an exponential and a polynomial of order p , and the most interesting cases for machine learning are $p = 3/2$ and $p = 5/2$, for which

$$\begin{aligned} k_{3/2} &= \left(1 + \frac{\sqrt{3}r}{l}\right) \exp\left(-\frac{\sqrt{3}r}{l}\right) \\ k_{5/2} &= \left(1 + \frac{\sqrt{5}r}{l} + \frac{\sqrt{5}r^2}{3l^2}\right) \exp\left(-\frac{\sqrt{5}r}{l}\right). \end{aligned}$$

Using standard algebraic manipulation, it is possible to evaluate the predictive distribution at the point y_{new} given the new features vector $\mathbf{x}_{new}$

$$P(y_{new}|\mathbf{y}, \mathbf{X}, \mathbf{x}_{new}) = N\left(h(\mathbf{x}_{new})^t \boldsymbol{\beta} + \mu, \sigma^2 + \Sigma\right), \quad (2.31)$$

where

$$\mu = K(\mathbf{x}_{new}^t, \mathbf{X}) (K(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathbf{I})^{-1} (\mathbf{y} - \mathbf{H}\boldsymbol{\beta}) \quad (2.32)$$

$$\Sigma = k(\mathbf{x}_{new}, \mathbf{x}_{new}) - K(\mathbf{x}_{new}^t, \mathbf{X}) (K(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathbf{I})^{-1} K(\mathbf{X}, \mathbf{x}_{new}^t) \quad (2.33)$$

with

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \in \mathbb{R}^{n \times 1}, \mathbf{f} = \begin{pmatrix} f(\mathbf{x}_1) \\ f(\mathbf{x}_2) \\ \vdots \\ f(\mathbf{x}_n) \end{pmatrix} \in \mathbb{R}^{n \times 1},$$

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^t \\ \mathbf{x}_2^t \\ \vdots \\ \mathbf{x}_n^t \end{pmatrix} \in \mathbb{R}^{n \times d}, \mathbf{H} = \begin{pmatrix} h(\mathbf{x}_1)^t \\ h(\mathbf{x}_2)^t \\ \vdots \\ h(\mathbf{x}_n)^t \end{pmatrix}, \in \mathbb{R}^{n \times p}.$$

$$K(\mathbf{X}, \mathbf{X}) = \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \cdots & k(\mathbf{x}_1, \mathbf{x}_n) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \cdots & k(\mathbf{x}_2, \mathbf{x}_n) \\ \vdots & \vdots & \vdots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & k(\mathbf{x}_n, \mathbf{x}_2) & \cdots & k(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

2.4.3 Artificial Neural Networks

Artificial neural networks (ANN), or simply **Neural Network (NN)**, take inspiration from how the human brain computes complex processes and, specifically, how neurons in our brains work. Similarly to our brain, an NN consists of many units called artificial neurons connected by edges (synapses in our analogy). Each neuron receives a signal from other neurons, processes it and then sends it to other connected neurons. The signal refers to a real number, and each neuron's output is determined by a nonlinear function applied to the sum of its inputs, known as the activation function. The strength of the signal at each connection is controlled by a weight, which is modified during the learning process. A basic feedforward neural network consists of many layers of neurons, and the output of the previous layer serves as the input to neurons in the next layer. Given a nonlinear activation function $f(\cdot)$ (e.g., ReLU, sigmoid, or tanh), a NN can be written as follows:

$$\hat{\mathbf{y}} = f(\mathbf{W}_L \cdot f(\mathbf{W}_{L-1} \cdot \dots \cdot f(\mathbf{W}_1 \cdot \mathbf{X} + \mathbf{b}_1) + \mathbf{b}_{L-1}) + \mathbf{b}_L) \quad (2.34)$$

where $\mathbf{X}$ is the input matrix of features $\in \mathbb{R}^{d \times n}$, $\mathbf{W}_L$ is the weight matrix associated to layer L , $\mathbf{b}_L$ the L layer bias. Training an NN means finding the weights $\mathbf{W}$ and biases $\mathbf{b}$ that minimise a loss function (e.g., Mean Squared Error for regression), gradient-based methods such as backpropagation are used. Roughly speaking, gradients of the loss function with respect to the weights are calculated, and the weights are updated iteratively with the following rule:

$$\mathbf{W}_{\text{new}} = \mathbf{W}_{\text{old}} - \eta \cdot \nabla L(\mathbf{W}) \quad (2.35)$$

where η is the learning rate and $\nabla L(\mathbf{W})$ is the gradient of the loss function L with respect to the weights W .

2.4.4 Stacked Regression

The predictions from the methods described above are used as input for the Stacked Regression. **Stacked Regression**, first introduced by Breiman [23], is an ensemble learning technique to combine multiple regression models via a meta-regressor. Stacking combines the strengths of individual estimators by using their outputs (i.e., predictions) as inputs for a final estimator. For example, in [261], Stacked Regression outperformed three ML models in downscaling ERA5 air temperature. The results presented in [23] demonstrated that Stacked Regression never performs worse than selecting the single best predictor, and that the greatest improvements occur when dissimilar sets of predictors are stacked. For example, stacking k different NNs is unlikely to yield significant improvement since the predictors are learning from the data in similar ways.

Care must be taken when implementing stacked regression, as an improper setup can lead to overfitting. As Breiman highlights, if the base estimators are trained on the entire dataset, the final estimator is likely to overfit the data. A common solution is to use cross-validated predictions: the dataset is divided into k folds, each base estimator is trained on the $k - 1$ folds, while the remaining fold is used to compute the predictions. In each iteration, the base estimators generate predictions for the fold that was not used during training, which are then collected across all iterations, stacked together, and then used as input for the final estimator.

Mathematically, the original Stacked Regression proposed by Breiman consists of finding $\hat{\beta}_h$ that minimises:

$$\sum_{n=1}^N (y_n - \sum_{h=1}^H \hat{\beta}_h \hat{f}_h(x))^2 \quad (2.36)$$

where H is the number of base estimators, $\hat{\beta}_h$ are the weights assigned to the predictions of the h -th base estimator, and $\hat{f}_h(x)$ is the prediction of the h -th base estimator for input X , i.e., the stacked estimator is the least squares. This has been generalised to include different types of estimators.

To clarify how Stacked Regression can be performed, algorithm 1 shows the pseudo-code used in this work to perform Stacked Regression, which, despite being used here, is not specific to this work. Here, the base estimators H are RF, GBT, GPR, and NN, while the final estimator G is the eXtreme Gradient Boosting (XGBoost) [35], an efficient and scalable implementation of the gradient boosting framework that has gained substantial popularity in recent years, largely due to its role in helping teams win nearly every Kaggle structured data competition.

Algorithm 1 Stacking with Cross-Validation

```
1: Input:
2:   Dataset  $D = \{(Y_i, X_i)\}_{i=1}^N$  where  $X_n$  is an input vector
3:   Number of folds  $V$  for cross-validation
4:   Number of base estimators  $H$ 
5: Step 1: Split the dataset into folds:
6:   Split  $D$  into  $V$  equal-sized folds  $D_1, D_2, \dots, D_V$ 
7: Step 2: Initialize prediction storage:
8:   Initialize an empty list to store predictions,  $\hat{S} = \{\hat{Y}_i^1, \hat{Y}_i^2, \dots, \hat{Y}_i^H\}_{i=1}^N$ .
9: Step 3: Train base estimators for each fold:
10:  for each fold  $v = 1, 2, \dots, V$  do
11:    Define training set  $D^{(-v)} = D - D_v$  and validation set  $D_v$ 
12:    for each model  $h = 1, 2, \dots, H$  do,
13:      Train the base estimator (level 0)  $M_h^{(-v)}$  on  $D^{(-v)}$ 
14:      Predict  $\hat{Y}_v^{(h)}$  using model  $M_h^{(-v)}$ 
15:      Store prediction  $\hat{Y}_v^{(h)}$  in  $\hat{S}(v, h)$ 
16:    end for
17:  end for
18: Step 4: Create level 1 learning sample:
19:   Create  $D_{CV} = \{(Y, \hat{S})\}$ 
20: Step 5: Train the final estimator (level 1 learner):
21:   Train the final estimator  $G$  (level 1 learner) on  $D_{CV}$ 
22: Step 6: Final prediction:
23:  for each new input  $X_i$  in test data  $X_{\text{test}}$  do
24:    for each model  $h = 1, 2, \dots, K$  do
25:      Predict  $\hat{Y}_i^{(k)}$  using base model  $M_h$ 
26:    end for
27:    Stack predictions into  $X_{\text{stacked\_test}} = (\hat{Y}_i^{(1)}, \hat{Y}_i^{(2)}, \dots, \hat{Y}_i^{(H)})$ 
28:    Predict final output using the final estimator  $\hat{Y}_i = G(X_{\text{stacked\_test}})$ :
29:  end for
30: Output: Final predictions  $\hat{Y}_{\text{test}}$  for test data
```



Chapter 3

IASI Implementation: from L1 to L3

This chapter describes the methodological framework adopted to generate gridded L3 LST and T_d from IASI radiances (L1). Section 3.1 details the implementation to retrieve the L2 geophysical parameters from L1 radiances, while Section 3.2 the machine-learning methodology employed to produce gap-filled and downscaled L3 products.

3.1 From L1 to L2

This section describes the procedure to retrieve the L2 geophysical parameters. Specifically, Section 3.1.1 introduces the two selected target areas in Italy, which have been severely affected by drought events over the past decade. Sections 3.1.2 and 3.1.3 present the implementation of the physical inversion procedure to retrieve L2 geophysical products from L1 IASI radiances, including the computation of T_d (Section 3.1.4).

3.1.1 Target Areas

The focus is on two Italian regions: the Po Valley region (northern Italy) and Basilicata region (southern Italy). Both districts have suffered over the past few years from seasonal drought, which has widely stressed the ecosystem and increased the risks of fires and other hazards.

The Po Valley region (44° to 46°N, 7° to 13°E WGS84) is located in northern Italy and covers an area of approximately 105 096 km². This large area contains the Alps, the Apennines, and the Po Valley plains showing strong differences in altitudes, vegetation cover, and climate. Figure 3.1 illustrates the region of interest, with land cover information based on the CORINE Land Cover (CLC) 2018 dataset, available at <https://land.copernicus.eu/pan-european/corine-land-cover>.

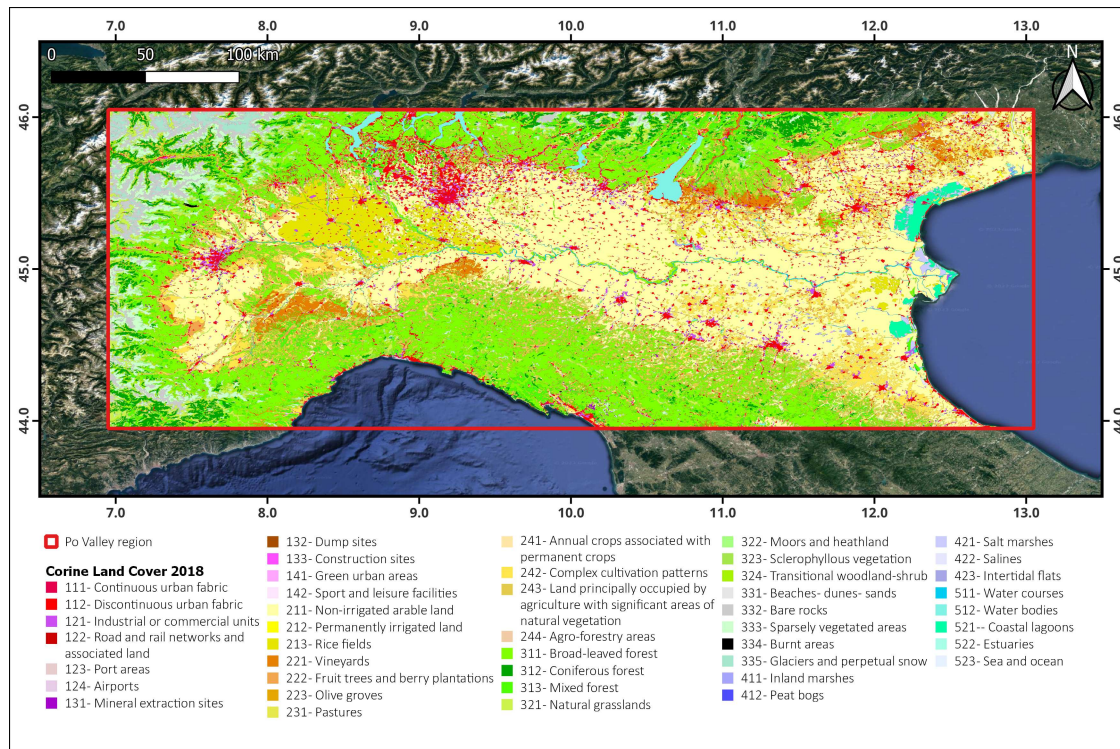


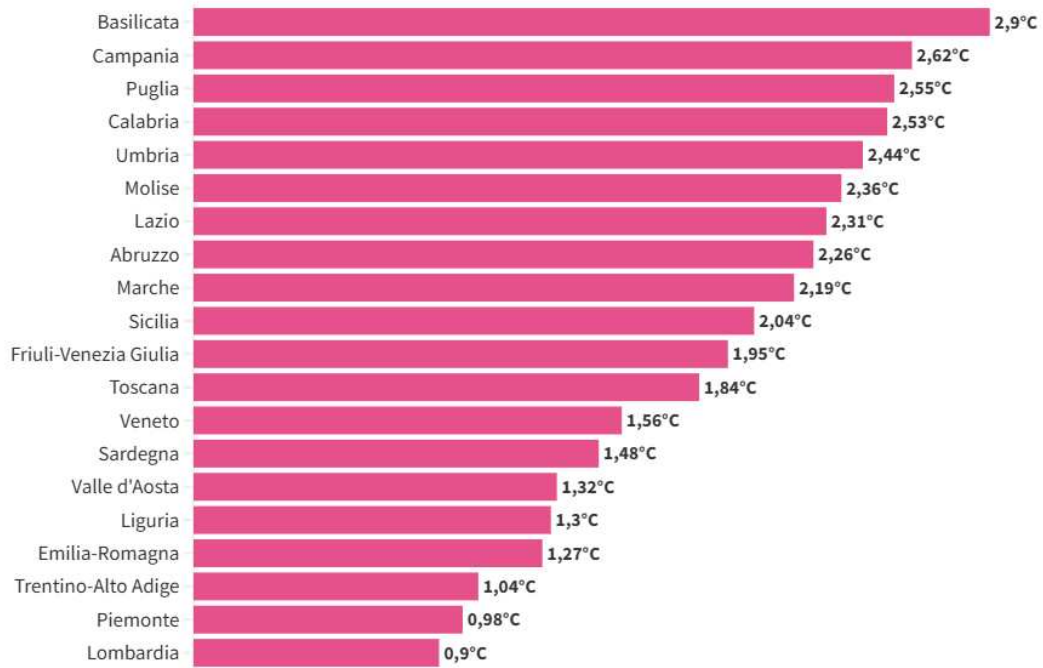
Figure 3.1: The red box indicates the Po Valley target region. The shapefile is the CLC 2018 providing information on the land cover.

The Po Valley region is a flat alluvial plain crossed by the Po River and highly devoted to agriculture. The plain is surrounded by the Apennines in the southern part and by the Alps in the northern and western parts. The Apennines, which rarely exceed 2000 m in altitude, extend 1200 km along the Italian peninsula, hosting a rich variety of flora and fauna. These areas contain some of Europe's best-preserved montane grasslands and forests, mainly composed of broad-leaved woodlands. In contrast, the Alps form Europe's largest and highest mountain range, with many peaks exceeding 4000 m and covered by broad-leaved and coniferous forests.

In 2022 northern Italy was severely affected by drought. The Po Valley experienced a precipitation deficit since the winter of 2021, a period of particular importance because precipitation in Mediterranean countries mostly occurs during winter. Higher-than-average temperatures combined with a persistent lack of rainfall triggered a significant drought in the region, further exacerbated by the incredible snowfall deficit over the Italian Alps (with an average snowfall deficit of 45% for the year). This resulted in an unprecedented hydrological drought with a -85% Po River discharge in July near the river delta [56]. In the last two decades, drought episodes in this region have become stronger in terms of frequency and duration [13, 168]. Moreover, climate projections for Northern Italy predict an increase in drought severity, especially in the Alpine area [12], posing a significant challenge for the Po Valley, historically highly devoted to agriculture.

On the other hand, Basilicata is an inland region located in southern Italy, where the Apennine chain and its forests occupy the central part of the area, while croplands extend across the eastern

part of the region, especially near the coast. Contrary to the Po Valley region, the territory of Basilicata is predominantly mountainous (47%) and hilly (45%), with only a small percentage of flat land (8%). It has a single large plain: the Metaponto Plain. Forests in Basilicata are heavily affected by drought events. For example the forest of San Paolo Albanese has been suffering from long-lasting drought-induced tree mortality [196], especially among oak trees, where more than 50% of the mature specimens showed symptoms of death, while about 15% died recently [39]. Basilicata, along with many inland south Italy regions, is one of the most affected areas by drought events. Several studies have shown that the region is affected by land degradation, confirming the presence of environmental conditions favourable to drought development [5]. For instance, in late 2024, parts of northern Basilicata experienced a severe precipitation deficit (meteorological drought) that reduced the drinking water supply to 39 municipalities [150] and also led to a hydrological and socioeconomic drought. In the same year, the Basilicata region recorded the highest air temperature anomaly in Italy with respect to the 1991–2023 mean, as shown in Figure 3.2.



Fonte: Copernicus

Figure 3.2: Air temperature anomalies in 2024 with respect to the 1991–2023 mean for the Italian regions. Source: Pagella Politica [200]

Since Basilicata is a relatively small region (10 073 km²), I extended the study area to include the neighboring regions of Campania, Puglia and a small portion of Calabria, defining a box with the following coordinates: 39.25° to 42°N, 13° to 18.75°E WGS84. This also provides a reference to surrounding areas which, although located at the same latitude, experienced less severe dry conditions. Figure 3.3 illustrates the region of interest, with land cover information based on the CLC 2018 dataset.

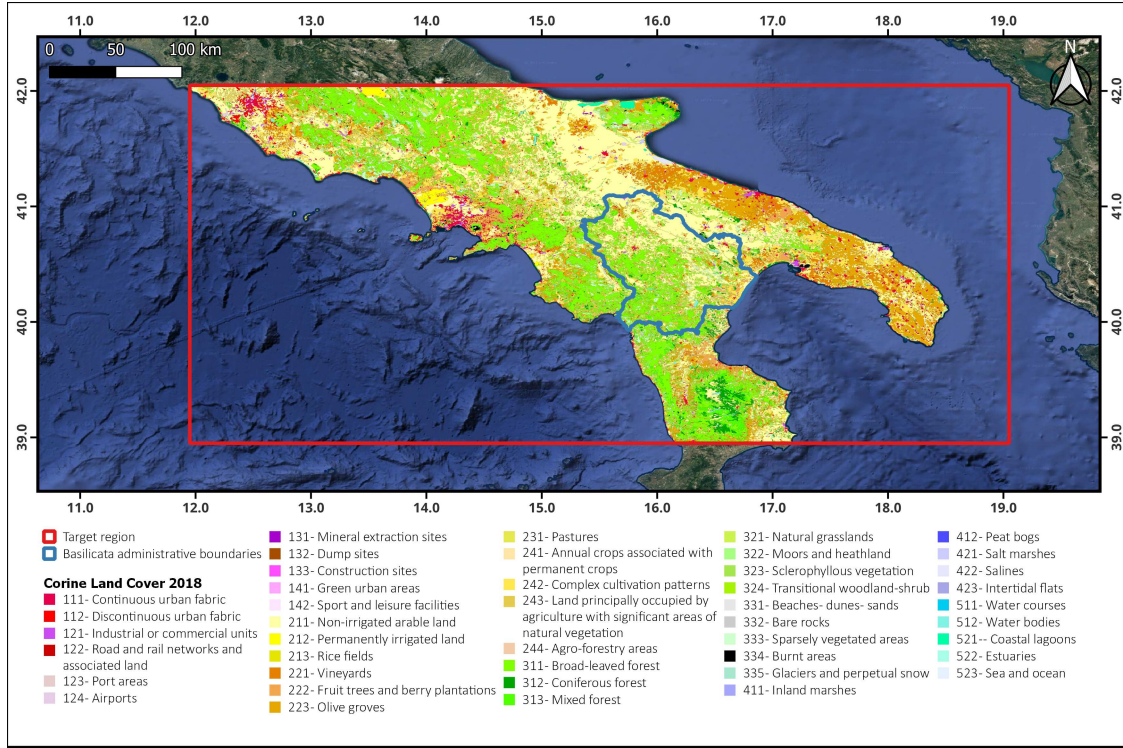


Figure 3.3: The red box indicates the target region that includes Basilicata. The shapefile is the CLC 2018 providing information on the land cover.

Both the areas exhibit a high degree of heterogeneity, and in a previous study [44], I have already shown that the response to heatwaves differs in magnitude between forested and cultivated areas. The objective of this thesis has been to develop a generalizable model able to provide reliable predictions at the global scale under different environmental conditions.

3.1.2 IASI Data

The LST and T_d were retrieved from the IASI sensor using IASI Level 1C data, downloaded from EUMETSAT at <https://navigator.eumetsat.int/product/EO:EUM:DAT:METOP:IASIL1C-ALL>. As described in Chapter 2, L1 products correspond to radiances measured by the instrument, which go through successive calibration and processing steps. EUMETSAT distinguishes between three types of L1 data: L1A, L1B, and L1C, but provides only the IASI Level 1C data. Table 3.1 highlights the differences between these three products. Through the EUMETSAT Data Access Client (EUMDAC), 10 years (from 2015 to 2024) of IASI data (Level 1C) over our two target regions were downloaded using the Python package available at <https://user.eumetsat.int/resources/user-guides/eumetsat-data-access-client-eumdac-guide> (more than 30,000 orbits coming from MetOp-A, MetOp-B, and MetOp-C platforms). Then, the orbits were converted into NetCDF format using the Data Tailor module.

Level	Description
Level 1A (L1A)	Radiometric post-calibration applied; spectral calibration provided (appended); geolocation using AVHRR/IIS co-registration. Spectra remain on the instrument's native (non-uniform) sampling.
Level 1B (L1B)	L1A spectra resampled to an equidistant wavenumber grid (oversampling and cubic-spline interpolation). Constant sampling, unapodized radiances.
Level 1C (L1C)	L1B spectra with apodization applied (IASI ISRF-based function). Effective spectral resolution $\sim 0.5 \text{ cm}^{-1}$; 8461 samples spanning 645–2760 cm^{-1} , with 0.25 cm^{-1} sampling.

Table 3.1: Summary of IASI Level 1 products (L1A, L1B, L1C).

3.1.3 Retrieval of Geophysical Products

For IASI retrieval, the atmospheric state vector included the surface temperature (T_{surf} in Kelvin (K)) and emissivity (ϵ_{surf}), atmospheric profiles of temperature (T , in K), and mixing ratio profiles of water vapour (H_2O in g/kg), isotopologues of water vapour (HDO in ppmv), ozone (O_3 in ppmv), carbon dioxide (CO_2 in ppmv), carbon monoxide (CO in ppmv), methane (CH_4 in ppmv), nitrous oxide (N_2O in ppmv), nitric acid (HNO_3 in ppmv), sulfur dioxide (SO_2 in ppmv), ammonia (NH_3 in ppmv), carbonyl sulfide (OCS in ppmv), and tetrafluoromethane (CF_4 in ppmv). The atmospheric profiles were specified on a fixed pressure (p) grid of $N_L = 60$ layers spanning the range 1050 hPa to 0.005 hPa. The pressure levels were labelled from 1 (ground) to $N_L + 1$ (Top of the Atmosphere), with an atmospheric layer bounded by two consecutive levels. The layer index goes from 1 to N_L . The first level pressure, p_1 is the surface pressure, p_{surf} ; the uppermost pressure level is $p_{N_L+1} = 0.005 \text{ hPa}$.

As regards emissivity, retrieval was not performed over sea surfaces ($T_{surf} = \text{Sea Surface Temperature (SST)}$); instead, Masuda's emissivity model [156] was applied. Over land, emissivity is represented through a truncated Principal Component (PC) analysis using 20 PC scores. The Principal Component Analysis (PCA) basis was built from the emissivity ensemble provided by the Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) Spectral Library version 2.0 [11] and the MODIS UCSB (University of California, Santa Barbara) Emissivity Library (<http://www.icesb.ucsb.edu/modis/EMIS/html/em.html>).

The ensemble was linearly resampled at the IASI sampling of 0.25 cm^{-1} and re-interpolated to the IASI range 645 to 2760 cm^{-1} , see [152, 155].

The total number m of parameters to retrieve from the inversion of the RTE Eq. 2.19 is given by $m = 1 + N_{\epsilon_{surf}} + 4 \times N_L + N_L \times N_G$, where the first addend refers to the Sea Surface Temperature (SST) or the Land Surface Temperature (LST), the second to surface emissivity and is equal to 0 for sea surface and to 20 for land (PC scores), the third to T , H_2O , HDO and O_3 , the last to the $N_G = 9$ gases.

Eq. (2.20), specified for IASI is the Gauss-Newton step that solves the linearized RTE with the

addition of the regularising term due to the prior knowledge Eq. (2.15)

$$R(i) = r_a(i) + \sum_{l=1}^{N_{\varepsilon_{surf}}} K_{\varepsilon_{surf}}(i, l)(c(l) - c_a(l)) + K_{T_{surf}}(i)(T_{surf} - T_{a, surf}) \quad (3.1)$$

$$\begin{aligned} & + \sum_{l=1}^{N_L} K_T(i, l)(T(l) - T_a(l)) + \sum_{l=1}^{N_L} K_{H_2O}(i, l)(H_2O(l) - H_2O_a(l)) \\ & + \sum_{l=1}^{N_L} K_{HDO}(i, l)(HDO(l) - HDO_a(l)) + \sum_{l=1}^{N_L} K_{O_3}(i, l)(O_3(l) - O_{3a}(l)) \quad (3.2) \\ & + \sum_{j=1}^{N_G} \sum_{l=1}^{N_L} K_{G,j}(i, l)(G_j(l) - G_{aj}(l)), i = 1, \dots, 8461 \end{aligned}$$

where the emissivity term $\sum_{l=1}^{N_{\varepsilon_{surf}}} K_{\varepsilon_{surf}}(i, l)(c(l) - c_a(l))$, with $\mathbf{c}$ vector of PC scores, is present only in case of retrieval over land. In the equation, 8461 is the total number of IASI channels, $N_L = 60$ is the number of atmospheric layers, $N_G = 9$ is the number of gaseous species, the subscript a denotes the *a priori* information both for atmospheric parameters and the radiance data and $\mathbf{K}$ is the Jacobian derivative with obvious meaning of subscripts.

Note that IASI does not have the spectral resolution and information content to retrieve the vertical profile of any of the N_G species listed above. For these gases, as shown in many previous IASI science studies, we have at most ≈ 2 degrees of freedom available. For this reason, the vertical profile was parameterised as a function of one free parameter, that is the column averaged amount alone. This is defined by

$$\bar{G}_j = \frac{1}{p_{surf}} \int_{p_{surf}}^0 G_j(p) dp \approx \frac{1}{p_{surf}} \sum_{l=1}^{N_L} G_j(p)(p(l) - p(l+1)) = \mathbf{h}^T \mathbf{G}_j \quad (3.3)$$

where G_j is the j -th generic mixing ratio (ppmv) of a generic gaseous species among CO_2 , N_2O , CO , CH_4 , SO_2 , HNO_3 , NH_3 , OCS , and CF_4 ; and $\mathbf{h}$ is the *averaging operator* whose elements were defined by

$$h_l = \frac{p(l) - p(l+1)}{p_{surf}}; l = 1, \dots, N_L.$$

Note that $G_j(l)$ is the layer average of the mixing ratio between the two levels l and $l+1$, therefore, the approximation formula for the integral is well balanced.

Let us consider the following scaling approximation

$$G_j(l) = (1 + f_j)(G_{aj}(l)), \text{ for each layer } l$$

where $G_{aj}(l)$ indicates the *a priori* information about gas j at layer l . Then in Eq. 3.1 the last term referred to gases simplifies to

$$\sum_{j=1}^{N_G} \sum_{l=1}^{N_L} K_{G,j}(i, l)(G_j(l) - G_{aj}(l)) = \sum_{j=1}^{N_G} f_j \sum_{l=1}^{N_L} K_{G,j}(i, l)G_{aj}(l) = \sum_{j=1}^{N_G} f_j K_{G,j}(i).$$

In this way, the retrieval problem considered the scaling factor f_j , and once calculated (i.e. $\hat{f}_j$) the estimated column-averaged amount was evaluated by

$$\bar{G}_j = (1 + \hat{f}_j)\bar{G}_{aj}. \quad (3.4)$$

Note that the column averaged amount is equivalent to what is commonly referred to as column amount expressed in ppv, because it is possible to show that $\hat{G}_j$ is the same as the ratio of the total column amount of the species j to the total column of dry air.

The complete forward/inverse processing chain for IASI data was implemented in a software package called ϕ -IASI, a FORTRAN-based inverse radiative transfer code for the optimal estimation of the thermodynamic state of the atmosphere. This package, which was recently updated to match the spectral coverage of the Far-infrared Outgoing Radiation Understanding and Monitoring (FORUM) mission [153], consists of two modules, the forward model, σ -IASI [9, 208] and the inverse one, δ -IASI [31, 152, 143, 207, 155, 29]. Reference [153] refers to the newest version of the code available upon request. The forward model is a pseudo-monochromatic, fast line-by-line radiative transfer scheme which computes the surface/atmosphere spectrum in the infrared and related Jacobian matrices. The core of σ -IASI is the RTE described in Chapter 2.2 valid for computing clear-sky radiances. The inversion of the RTE and the full IASI spectrum (8461 spectral channels) was performed using δ -IASI, which implements the retrieval scheme described in Chapter 2.3.

The computational complexity of Eq. 3.1 is 8461×270 for land retrieval and 8461×250 for sea. To reduce the computational cost associated with evaluating the SVD at each iteration, [207] proposed a statistical technique based on random projections to reduce the dimensionality of the radiance data. The radiative transfer equation was then solved in this reduced space for the retrieval of geophysical parameters. This approach enabled the assessment of IASI's capability to retrieve the OCS vertical profile, which was subsequently incorporated into the final version of the code, see [29]. As a result, the computational complexity of Eq. 3.1 was reduced to 1200×330 for land retrieval and 1200×310 for sea, where 1200 corresponds to the number of random components retained after projection.

The resolution of Eq. 2.20 requires both the observational covariance matrix $\mathbf{S}_\epsilon$, Eq. 2.14, and the prior information, Eq. 2.15.

As regards $\mathbf{S}_\epsilon$, since the IASI L1C spectra are Gaussian apodised [8] the IASI radiances are correlated and the related covariance matrix has off-diagonal terms, due to mechanical microvibrations of the beam splitter of the IASI instrument [210].

However, when using random projection, the observational covariance matrix of the radiances becomes diagonal. Moreover, both instrument and forward model errors can be incorporated into a single additive variance term. For mathematical details, see [29].

The prior information Eq. 2.15 was specified as follows:

- For emissivity over land, the a priori information (background) and the first guess are not the same. Specifically, the background, calculated as the mean of an ensemble of

states derived from ASTER and MODIS, may deviate significantly from the true emissivity state. As a result, it may fall outside the linear region surrounding the true state vector, potentially leading to a large number of iterations for convergence or even failure to converge. To mitigate this issue, the emissivity first guess was instead derived from the University of Wisconsin (UW) Baseline Fit (BF) Emissivity database (UW/BFEMIS database, e.g., <http://cimss.ssec.wisc.edu/iremiz> [204]). The method used to generate the emissivity first guess, ensuring spectral coverage and sampling consistent with IASI, is detailed in [154]. The covariance matrix of the PC scores is diagonal with elements equal to the singular values. Thus, for the background matrix of the 20 PC scores was used a diagonal matrix of size 20×20 with the diagonal elements set to the first 20 eigenvalues.

- for the atmospheric parameters and surface temperature ($T_{surf} = \text{LST}$), the state vector was made up of the time and space co-located ECMWF analyses for $(T_{surf}, T, \text{H}_2\text{O}, \text{O}_3)$. The covariance matrix was spatially localized and built up from a suitable ensemble of states derived from the ECMWF model.
- the background for HDO was obtained from that for H_2O , multiplying the latter vector by the abundance ratio $\text{HDO}/\text{H}_2\text{O}$ prescribed in the Standard Reference Material Vienna Mean Ocean Water (VSMOW), that is $R_{VSMOW} \approx 3.1 \times 10^{-4}$. In the same way the covariance matrix was scaled by R_{VSMOW}^2 .
- for all gases, the background column averaged amount was taken from climatology, assuming a time-constant background. The corresponding values are reported in Table 3.2.

Table 3.2: Background average column amount for each gas adapted from [143]. The values in brackets are the percentage error assumed for the background.

Gas	Background average column amount
CO	109.65 ppbv
CO ₂	397 ppm
N ₂ O	296.52 ppbv
CH ₄	1582 ppbv
SO ₂	134 pptv
HNO ₃	473 pptv
NH ₃	211 pptv
OCS	510 pptv
CF ₄	88.80 pptv

3.1.4 Computation of T_d

From the profiles of T and H_2O , only the elements corresponding to the lowermost atmospheric layer, denoted T_1 (in units of K) and $(\text{H}_2\text{O})_1$ (in units of g/kg), were considered. The corresponding layer pressure is denoted by P_1 (in units of hPa). The computation of T_d involves the calculation

of the actual water vapour pressure (P_w) and saturation water vapour pressure (P_{ws}) [151]. From $(\text{H}_2\text{O})_1$, P_w was computed according to:

$$P_w = 10^{-3} P_1(\text{H}_2\text{O})_1 \frac{R_w}{R_{\text{air}}} = b P_1(\text{H}_2\text{O})_1, \quad b = 10^{-3} \frac{R_w}{R_{\text{air}}} \quad (3.5)$$

with P_w in hPa, where $R_w = 461.5 \text{ J}/(\text{kg K})$ and $R_{\text{air}} = 286.9 \text{ J}/(\text{kg K})$ are the specific gas constants of water vapour and air, respectively. According to [98], P_{ws} was computed as:

$$P_{ws} = 10^{-2} \exp \left[\frac{a_1 - a_2}{t_1 + a_3} \right] (t_1 + a_4)^{a_5} \quad (3.6)$$

with $t_1 = T_1 - 273.15$ (temperature in $^{\circ}\text{C}$) and P_{ws} in hPa. Eq. (3.6) is valid for $t_1 > 0$ (vapour pressure of water), where $a_1 = 34.494$, $a_2 = 4924.99$, $a_3 = 237.1$, $a_4 = 105$, and $a_5 = 1.57$ are fit parameters. From Eq. (3.5) and (3.6), the fractional relative humidity rh has been obtained as:

$$rh = \frac{P_w}{P_{ws}}, \quad (3.7)$$

whose value permits the final evaluation of T_d (in $^{\circ}\text{C}$) by using the Magnus formula [214] as follows:

$$T_d = \frac{cx}{b - x} \quad \text{with} \quad x = \ln(rh) + \frac{bt_1}{c + t_1}, \quad (3.8)$$

where t_1 is the temperature of the lowermost atmospheric layer (in $^{\circ}\text{C}$), $b = 17.62$ (dimensionless), and $c = 243.12^{\circ}\text{C}$.

3.2 From L2 to L3

This section describes the proposed **downscaling–fusion methodology**, designed to reconstruct missing LST and T_d values over spatial fields derived from spatially scattered IASI observations, producing regularly gridded (L3) data. Specifically, Section 3.2.1 provides background information on the interpolation techniques proposed for reconstructing LST and T_d . Sections 3.2.2 and 3.2.3 describe the interpolation workflow for LST and T_d , respectively. Finally, Sections 3.2.4 to 3.2.6 present the actual implementation of the methodology.

3.2.1 Background

IASI L2 products were retrieved following the sensor viewing geometry, i.e. independently for each pixel of the target regions and every single day of the considered period. Unfortunately, since IASI is an infrared sensor, it cannot penetrate thick cloud layers leading to reliable retrievals only in clear-sky pixels. Indeed, the ϕ -IASI package automatically discards cloudy pixels using the internal Advanced Very-High-Resolution Radiometer (AVHRR) cloud mask; pixels with a cloud fraction greater than 5% were removed. This introduces missing data, requiring an interpolation step to transform the sparsely populated, non-uniform L2 observations (the ϕ -IASI output) into evenly gridded maps. Spatial interpolation in remote sensing is becoming increasingly important

and widespread. A search on Scopus using the keywords "Spatial Interpolation" and "Remote Sensing" returned more than 1,000 published articles, with the number constantly increasing year by year (see Figure 3.4). However, remote sensing is a broad field, and in this work the focus is

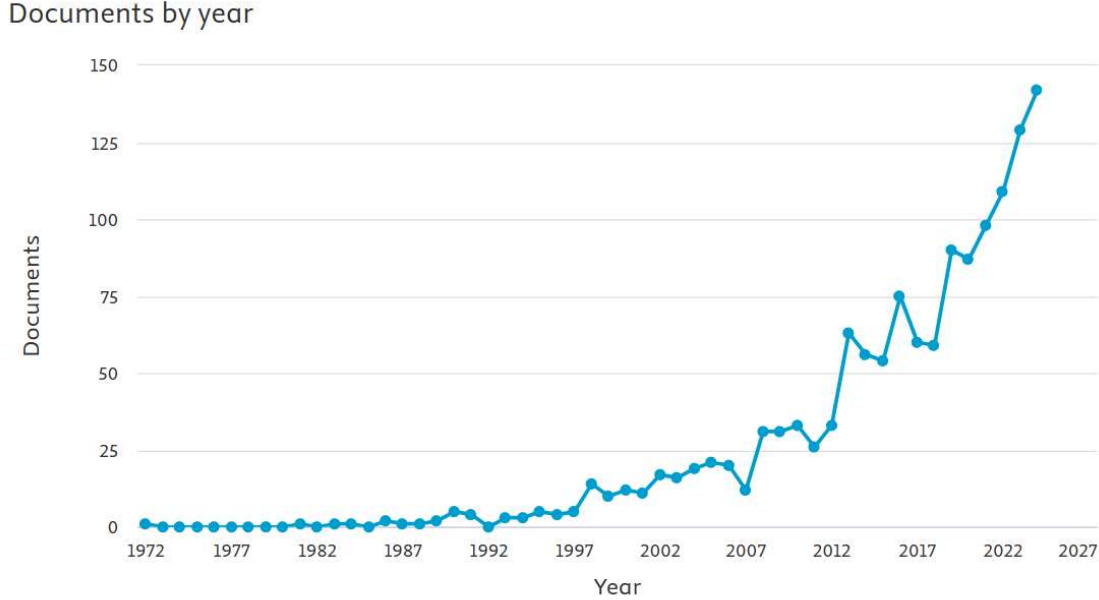


Figure 3.4: Number of published articles per year on Scopus using the keywords "Spatial Interpolation" and "Remote Sensing".

specifically on LST and T_d .

Regarding the latter, no articles were found that are strictly related to the interpolation of T_d .

Conversely, many studies have focused on interpolation and downscaling of LST products to produce high-resolution LST data [190]. Given the heterogeneity of LST and its relationship to several types of environmental factors such as land cover, topography, soil moisture, incoming solar radiation, and wind speed [137, 222], ML algorithms are becoming increasingly popular due to their ability to model this nonlinear relationship. For example, [104, 133, 51, 249, 252, 134, 131] proved that a simple RF model can outperform many other ML and NN algorithms in downscaling LST images from MODIS. In [133], the authors reached a final resolution ten times more detailed than the original one (from 990 m to 90 m) with an RMSE of around 2 K. Deep Learning has been used in LST downscaling, like with Convolutional Neural Network (CNN) [176], geographically weighted neural network regression (GNNWR) [139], and Multi-layer Perceptron (MLP) [37, 83].

However, almost all the above-cited studies focus on downscaling LST images from MODIS (see also [50]) and from other sensors, such as AVHRR [38, 216], ASTER [245, 96], LANDSAT [198, 47, 246, 2, 178, 217], SEVIRI [256, 123], or GOES [128]. See [190] and references therein.

To the best of our knowledge, the downscaling of LST products generated from IASI data has not yet been addressed. Some efforts have been made to retrieve regularly gridded LST using

Deep Neural Networks. For example, [202] presented an LST product obtained by applying a NN to radiances. However, to improve the results, they incorporated a monthly surface emissivity product, and the predicted LST values were subsequently interpolated. Other examples are described in [3, 22, 21] where localized CNNs were tested to predict LST directly from radiances. Since CNNs operate on images, the authors converted the L1 products into regular grid images at 0.2° resolution. However, missing data are still present, making an inter-/extrapolation algorithm based on PCA necessary to facilitate smooth training.

In [43], a method similar to the Gaussian Optimal Interpolation approach was proposed, using background data to produce monthly maps from L2 observations at 0.05° resolution. However, this procedure, which was already tested on many surface and atmospheric parameters [151, 209, 44, 185], generated maps that are quite smoothed. Although this approach is perfectly suitable for parameters like gases, which typically show little variation over short distances, it does not hold true for LST and, to a lesser extent, T_d , both of which can vary significantly.

For this reason, the **downscaling–fusion methodology** described in Section 2.4 was applied. To account for seasonal variability, the workflow was implemented on a monthly basis, training a separate model for each month and for each ML algorithm. The models were developed to predict LST and T_d at the locations of the L2 satellite observations, using a set of covariates derived from other satellite sensors, vegetation products, reanalysis datasets, and territorial and geographic information. All input datasets were spatially and temporally co-located with the L2 observations to ensure consistency. Subsequently, the predicted LST and T_d fields were downscaled by exploiting the higher spatial resolution of the covariates, producing estimates over a regular 0.05° grid, thereby effectively doubling the spatial resolution of the original data.

3.2.2 LST Interpolation

To retrieve gap-filled and downscaled LST, the ML algorithm applied here takes advantage of a proxy of covariates related to the LST. These included LST from other sensors, vegetational products, and territorial and geographic information.

Geographical Covariates: DEM and CLC

Spatial dependence in the machine learning models was accounted for by including the spatial coordinates (latitude and longitude) as additional input features. Moreover, the European Digital Elevation Model (DEM) and the CLC 2018 dataset were used to better represent territorial characteristics. The DEM (<https://land.copernicus.eu/imagery-in-situ/eu-dem>) is provided as a raster at a spatial resolution of 25 m, while the CLC (<https://land.copernicus.eu/pan-european/corine-land-cover>) is distributed as a vector shapefile. Following the approach described in [44], the CLC dataset was converted into raster format at a spatial resolution of 100 m and simplified into five main classes corresponding to the Level 1 CLC classification: artificial surfaces, agricultural areas, forest and semi-natural areas, wetlands, and water bodies. A more detailed classification was found to reduce model performance, as spatial co-location becomes challenging when assigning a single detailed

CLC class to pixels with a minimum diameter of 12 km. It should be noted that Copernicus also provides a CLC product in raster format at a 100 m resolution. However, this dataset is generated by rasterizing the seamless European CLC vector dataset using the cell center method (<https://desktop.arcgis.com/en/arcmap/latest/tools/conversion-toolbox/how-polygon-to-raster-works.htm>). LST varies significantly across different land cover types [105, 226], as each category exhibits distinct thermal properties influencing heat absorption and emission. The LST retrieved by IASI represents an area of approximately 12 km in diameter, thus averaging the signal from a wide variety of land cover types. Unlike the cell center method, our approach assigns to each pixel the CLC class with the largest areal coverage, providing a more representative characterization of surface conditions within the IASI footprint.

Vegetational Covariates: LAI, FVC, and NDVI

It is well established that healthy vegetation mitigates LST and near-surface air temperatures by modifying surface albedo, enhancing evapotranspiration, and providing shade [103, 46, 119, 48]. Evapotranspiration converts solar energy into latent heat, thereby reducing air temperature and, consequently, LST. A dense vegetation canopy not only enhances shading—resulting in lower air temperatures and LST—but also promotes water retention beneath the canopy, leading to higher air humidity and greater moisture availability, which together contribute to a stronger cooling effect [260]. There is, therefore, a clear relationship between vegetation indices and LST, which can be exploited to improve the downscaling process, as demonstrated by [70]. In this work, three vegetation indices were employed as covariates: the Leaf Area Index (LAI), Fraction Vegetation Cover (FVC), and Normalized Difference Vegetation Index (NDVI). LAI quantifies the thickness of the vegetation canopy and is defined as half of the total one-sided area of green canopy elements per unit of horizontal ground area. FVC represents the fraction of the ground surface covered by green vegetation, thus quantifying the spatial extent of vegetation. NDVI is a widely used index for assessing vegetation health and density, based on the difference between near-infrared reflectance (strongly reflected by vegetation) and red reflectance (strongly absorbed by vegetation). The vegetation products were obtained from the MetOp LSA SAF dataset (<https://landsaf.ipma.pt/en/data/products/vegetation/>), with a temporal resolution of 10 days and a spatial resolution of 1 km ($\approx 0.0089^\circ$). These products are derived from the AVHRR sensor, an across-track scanner onboard the MetOp platforms, which also host the IASI instrument. Only high-quality pixels were retained following the recommendations of the LSA SAF Product User Manual (<https://nextcloud.lsasvcs.ipma.pt/s/sWn23j9NZnJg2a6>). Observations flagged for poor quality (bit 7 = 1), large estimation errors ($FVC_ERR > 0.2$, $LAI_ERR > 1.5$), or excessive observation age ($Z_Age > 15$)—typically associated with snow cover or persistent cloudiness—were discarded.

Other LST Products: SEVIRI and AVHRR

To further improve the quality of the final predictions, two additional LST products were incorporated: one derived from the AVHRR sensor and the other from the SEVIRI sensor. Both LST datasets were obtained from the LSA SAF platform (<https://lsa-saf.eumetsat.int/en/data/products/land->

surface-temperature-and-emissivity). The temporal and spatial resolutions of the products are 15 minutes and 0.05° for the LST SEVIRI product, and 12 hours (day and night) and 0.01° for the LST AVHRR product, respectively. Only pixels with nominal or above-nominal quality—corresponding to LST uncertainties below 2 K—were retained. This uncertainty threshold represents a trade-off, ensuring the selection of high-quality LST values while maintaining a sufficient number of data points for validation purposes.

Model

The regression model used to solve for LST interpolation was the following:

$$LST_{IASI} = f(lat, lon, minutes, DOY, year, DEM, LST_{SEVIRI}, LST_{AVHRR}, CLC, LAI, FVC, NDVI) \quad (3.9)$$

where:

- *lat, lon*: latitude and longitude ($^\circ$)
- *minutes*: acquisition time in minutes (1--1440)
- *DOY*: day of year (1--365)
- *year*: acquisition year
- *DEM*: Digital Elevation Model (m)
- *LST_{SEVIRI}, LST_{AVHRR}*: LST products from SEVIRI and AVHRR sensors ($^\circ\text{C}$)
- *CLC*: Corine Land Cover class
- *LAI, FVC, NDVI*: vegetation indices derived from AVHRR

LAI and FVC were removed during the winter months (from November to April) because they provided little useful information: in winter vegetation growth is largely absent, resulting in low and uninformative values. Therefore, the resulting equation is:

$$LST_{IASI} = f(lat, lon, minutes, DOY, year, DEM, LST_{SEVIRI}, LST_{AVHRR}, CLC, NDVI) \quad (3.10)$$

3.2.3 T_d Interpolation

Similarly to LST, the retrieval of gap-filled and downscaled T_d uses the same ML algorithm but applied to a different set of covariates. These include atmospheric parameters and territorial and geographic information.

Geographical Covariates: DEM and CLC

Same as Section 3.2.2.

Atmospheric Covariates: ERA5 Products

Unlike LST, T_d is an atmospheric parameter and therefore it is more difficult to identify suitable covariates. As with LST, where additional LST products were included to improve interpolation accuracy, five atmospheric covariates derived from the ERA5-Land hourly dataset [172] were incorporated: air temperature at 2 m ($T_{air_{ERA5}}$), dew-point temperature at 2 m ($T_{d_{ERA5}}$), wind speed at 2 m ($WIND_{ERA5}$), total evaporation ($EVAP_{ERA5}$) and surface solar short-wave radiation downwards ($Down_shortwave_{ERA5}$). Total evaporation refers to the accumulated amount of water that has evaporated from the Earth's surface, including a simplified representation of transpiration (from vegetation), into water vapour in the air above. Surface solar short-wave radiation downwards is the amount of solar radiation (shortwave radiation) reaching a horizontal plane at the Earth's surface and includes both direct and diffuse components. Wind speed is not directly available in the ERA5-Land dataset; instead, it is provided as two components: the eastward (10 m) u-component and northward (10 m) v-component, both measured at a height of ten metres above the surface. These two components were first adjusted to the standard 2 m height to ensure consistency with the ERA5 air and dewpoint temperature levels. Assuming a short grass surface as a general approximation, the adjustment was performed using the following empirical formula [7]:

$$u(z_2) = u(z_{10}) \frac{4.87}{\ln(67.8z - 5.42)} \quad (3.11)$$

where z is the height of the measurement to be converted (10 m in this case), $u(z_2)$ is the wind speed at 2 m, $u(z_{10})$ is the wind speed at $z = 10$ m. Finally, the total wind speed was computed from the two components using the Pythagorean theorem: $Wind\ speed = \sqrt{U^2 + V^2}$.

Model

The regression model used to solve for T_d interpolation was the following:

$$T_{d_{IASI}} = f(lat, lon, minutes, DOY, year, DEM, T_{d_{ERA5}}, T_{air_{ERA5}}, WIND_{ERA5}, EVAP_{ERA5}, Down_shortwave_{ERA5}) \quad (3.12)$$

where:

- lat, lon : latitude and longitude ($^\circ$)
- DOY : day of year (1–365)
- $minutes$: acquisition time in minutes (1–1440)
- $year$: acquisition year
- DEM : Digital Elevation Model (m)

- Td_{ERA5} : ERA5-Land dew point temperature at 2 m (K)
- $Tair_{ERA5}$: ERA5-Land air temperature at 2 m (K)
- $WIND_{ERA5}$: ERA5-Land wind speed at 2 m
- $EVAP_{ERA5}$: ERA5-Land total evaporation (m of water equivalent)
- $Down_shortwave_{ERA5}$: ERA5-Land surface solar short-wave radiation downwards (J/m^2)

3.2.4 Implementation

Section 2.4 introduced the mathematical foundations of the interpolation step. The methodology relies on a set of base learners—RF, GBT, GPR, NN—which are subsequently combined using Stacked Regression. Section 2.4.4 presented a generic pseudo-algorithm for this procedure. However, while that framework served as a reference, the implementation adopted in this study is more complex and refined than the generic one.

Although the analysis covers relatively large areas, adequate spatial coverage can only be achieved by focusing on **monthly products**. This approach is consistent with previous studies [43, 151, 209, 44, 185], which demonstrated that IASI L2 observations alone are insufficient to achieve both a finer spatial resolution (0.05°) and a temporal frequency higher than the monthly scale. Instead of training a single large model, a set of models was developed to account for seasonal variability and the differences between daytime and nighttime satellite overpasses. The dataset includes two sensing times—day and night—separated by approximately 12 hours, corresponding to satellite ground tracks at approximately 09:30 and 21:30 local time, respectively. Owing to the sensor’s viewing geometry, the actual acquisition times extend over a broader time window. Figure 3.5 illustrates the distribution of IASI acquisition times for both day and night overpasses across the two target regions, indicating an effective time window of approximately two hours.

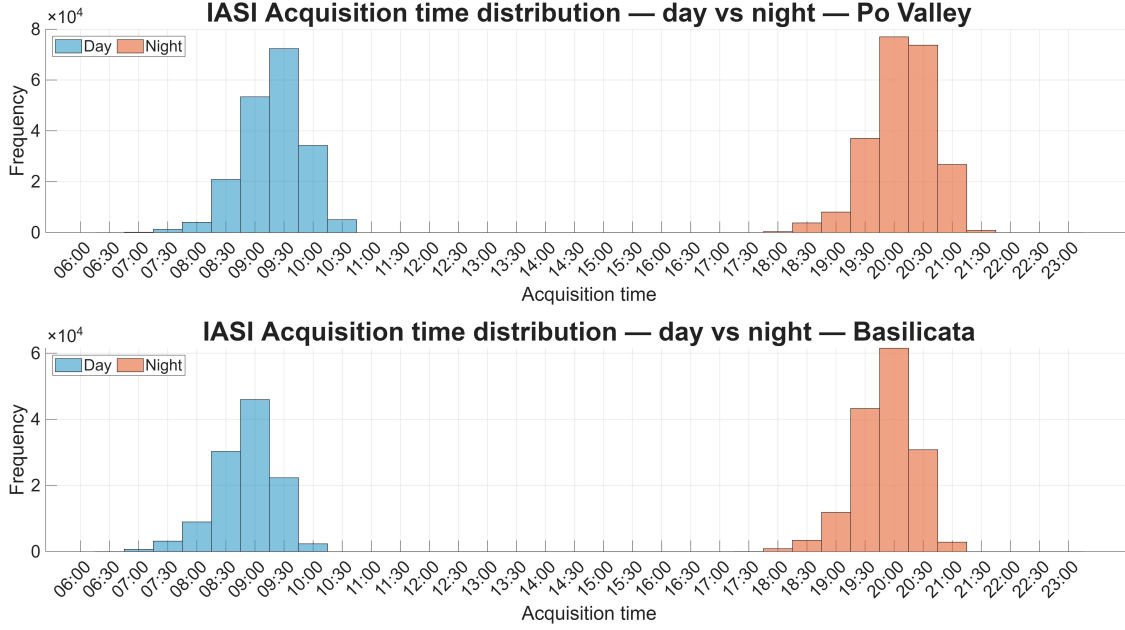


Figure 3.5: Distribution of IASI acquisition times in the Po Valley (top) and Basilicata (bottom).

These daytime and nighttime overpasses capture distinct thermal regimes. The 09:30 overpass corresponds to the morning warming phase, when surface and air temperatures rise under increasing solar radiation, whereas the 21:30 overpass occurs during the evening cooling phase, when temperatures decrease as the surface loses heat through longwave radiation.

To further account for seasonal variability, separate models were trained for each month. This strategy eliminates the need to explicitly include the month variable as a feature, thereby allowing the machine learning algorithm to focus on learning spatial and temporal patterns specific to each period.

In summary, for each target region, one model was developed for each month and for each overpass, resulting in a total of 24 models per target region. The following sections describe the construction of the datasets and the implementation of the ML framework in detail. Section 3.2.4 explains the spatial and temporal co-location of the covariates with the IASI L2 observations, Section 3.2.5 details the model training procedure, and Section 3.2.6 describes the generation of the L3 maps. The workflow is identical for LST and T_d , with the only difference being the selection of covariates used in each case.

Spatial and Temporal Co-location

All downloaded and preprocessed datasets were spatially and temporally co-located with the IASI L2 observations to construct the L2 training dataset.

As discussed in Section 2.1, each IASI observation has a spatial resolution of approximately 12 km at nadir, which can extend to more than 20 km for off-nadir observations. Furthermore, the IASI footprint is circular only at nadir and becomes progressively elongated and elliptical toward the swath edges. Therefore, accurately representing the footprint geometry was essential.

The Field Of View (FOV) angle (also referred to as the *pixel zenith angle*) alone does not provide sufficient information to fully determine the footprint shape, as the orientation of the ellipse’s major and minor axes depends on the satellite’s orbital geometry. Determining this orientation requires precise orbital data, which adds considerable complexity to the co-location process. To simplify the processing, the elliptical footprint was approximated by a circle with a diameter equal to its minor axis. This conservative approximation ensures that the circular area remains entirely contained within the true footprint. For **spatial co-location**, the covariates—available at a finer spatial resolution than IASI—were averaged within each IASI footprint. In the case of the CLC dataset, which represents a categorical variable, the most frequent class within each footprint was assigned to that footprint.

Particular attention was given to **temporal co-location**, as the selected covariates exhibit differing temporal resolutions. For the vegetation indices (LAI, FVC, NDVI) and LST_{AVHRR} , which have temporal resolutions of ten days and one day, respectively, the observation closest in time to the IASI acquisition date was used. Conversely, for the ERA5-Land and LST_{SEVIRI} products, which have temporal resolutions of one hour and fifteen minutes, respectively, the observations temporally closest to the exact IASI acquisition time were selected. Figure 3.6 illustrates an example of the spatial and temporal co-location between IASI and AVHRR LST observations.

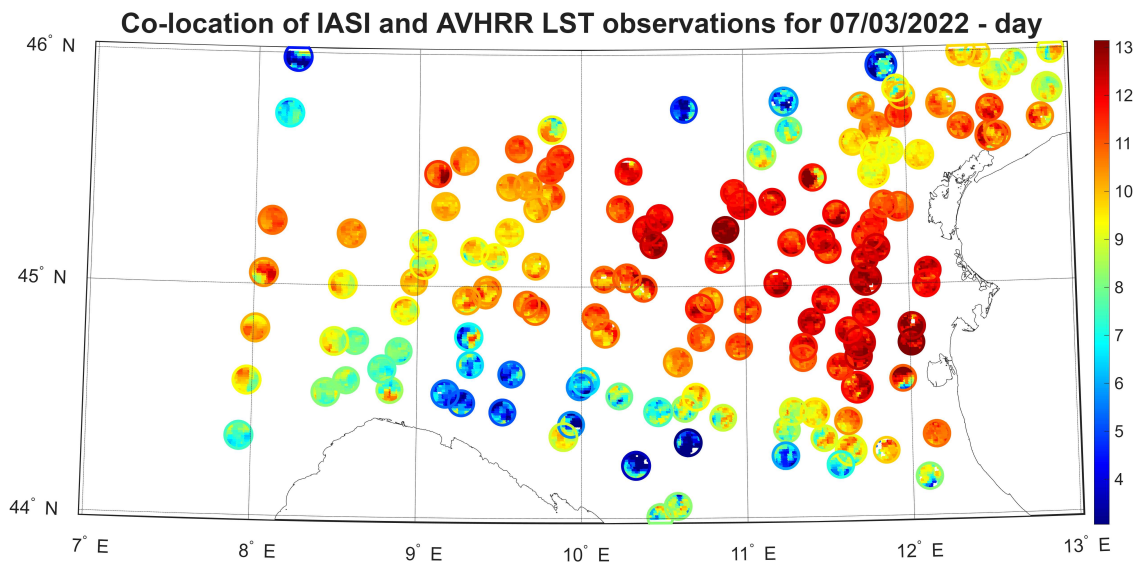


Figure 3.6: Example of co-location between IASI and AVHRR LST on 07/03/2022 (day passage). The circles represent the IASI footprints. AVHRR LST pixels falling within each footprint are shown inside the circles, and the circle edge color indicates the LST value assigned to that IASI footprint (i.e., the mean of the enclosed AVHRR pixels).

Finally, a **preprocessing step** was applied to clean the training dataset from missing values and outliers. For LST, outliers were detected by comparing the IASI LST values with the corresponding measurements from the two other LST products, while for T_d , outliers were identified by comparing the IASI T_d values with those from ERA5. This filtering step was crucial, as several pixels exhibited discrepancies exceeding 10°C , which could adversely affect model performance.

Specifically, for each month, the Interquartile Range (IQR) method was applied to the linear differences between the reference products (LST AVHRR, LST SEVIRI, ERA5 T_d) and the corresponding IASI measurements, rather than to the individual IASI values. Outliers were defined as any values falling outside the range:

$$(Q_{25} - 3 \times \text{IQR}) \text{ to } (Q_{75} + 3 \times \text{IQR}), \quad (3.13)$$

where

$$\text{IQR} = Q_{75} - Q_{25}. \quad (3.14)$$

An IQR multiplier of 3 was selected to remove only the most extreme outliers while retaining the majority of valid observations. This approach strikes an effective balance between filtering anomalous values and preserving valuable data for model training.

3.2.5 Training

The training dataset constructed in Section 3.2.4 was used as input to the stacked regression framework (Algorithm 1). For each target variable (either LST or T_d), together with the corresponding formulation and temporal information (day or night), the training dataset was subset accordingly and provided as input to the model training stage. The overall training procedure consisted of four main steps:

1. **Hyperparameter optimisation** — determination of the optimal configuration for each base learner using V-fold cross-validation and Bayesian optimisation applied to the entire training set.
2. **Training and prediction of base estimators** — independent training of each base learner to generate first-level predictions. Specifically, the training dataset was divided into five folds. The base estimators were trained on four folds using the hyperparameters determined in Step 1, while the remaining fold was used for validation. At each iteration, the validation predictions were concatenated into a single vector.
3. **Training of the final estimator** — combination of the base estimators' outputs using stacked regression to produce the final model. The predictions obtained from Step 2 were used as input features for the meta-learner (XGBoost). A dedicated hyperparameter optimisation procedure was also applied to the XGBoost model.
4. **Computation of L2 residuals for residual correction** — evaluation and correction of systematic biases in the model predictions through the computation of L2 residuals.

All ML models were trained in MATLAB (R2024b) using the following functions: `fitensemble` for RF and GBT, `fitrgp` for GPR, and `fitrnet` for NN. XGBoost is not natively implemented in MATLAB; however, the C++ implementation described in [229] was adapted for regression tasks, since the original version only supported classification.

For RF and GBT, the number of trees, the maximum number of decision splits (branch nodes), the minimum number of observations per leaf node, and the learning rate (only for GBT) were optimised.

For the NN, a more rigorous approach was adopted based on the formula proposed in [97] for a two-hidden-layer neural network with m output neurons and N training samples. The sufficient number of neurons in the first hidden layer was defined as $\sqrt{(m+2)N} + 2\sqrt{N/(m+2)}$, and in the second layer as $m\sqrt{N/(m+2)}$. In this study, 300 neurons were used in the first hidden layer and 60 in the second hidden layer.

For the GPR, the Matérn 3/2 kernel was used as the covariance function.

For XGBoost, the learning rate, maximum tree depth, minimum child weight, and number of parallel trees were optimised.

3.2.6 Prediction of L3 Products

To predict LST and T_d on the 0.05° L3 grid, the models trained in Section 3.2.5 were applied to an L3 dataset (hereafter referred to as the test dataset) constructed at the same spatial resolution. The test dataset was constructed following an approach similar to that described in Sections 3.2.4 and 3.2.5.

For **spatial co-location**, instead of using IASI footprints, the grid cells of a 0.05° regular grid covering the two target regions were employed, resulting in a total of 4961 pixels for the Po Valley and 6496 pixels for the Basilicata region. All covariate values were averaged within each 0.05° grid cell to match the target resolution. This approach is feasible because nearly all covariates have a spatial resolution equal to or finer than the target grid, with the only exception being the ERA5 covariates, which have a native resolution of 0.10° . In this case, rather than assigning the same value to the four 0.05° pixels contained within a single 0.10° ERA5 cell, a linear interpolation was applied to reach the target resolution using the Matlab's `griddedInterpolant` function.

Regarding **temporal co-location**, the high temporal resolution of the covariates was exploited to construct a daily test dataset. A temporal co-location strategy similar to that described in Section 3.2.4 was implemented, with the following adaptations:

1. For each day, the minimum, maximum, and mean acquisition times corresponding to the IASI observations were computed.
2. The mean acquisition time was used as a reference for all covariates, except for LST_{SEVIRI} , for which the minimum and maximum acquisition times were applied, averaging all observations within this temporal window.
3. The day of acquisition was assigned to the *Day of Year (DOY)* variable, and the mean acquisition time was assigned to the *minutes* variable.

Pixels containing missing values were removed from the dataset.

Subsequently, the base estimators trained on the entire training dataset (Step 1 in Section 3.2.5) were used to compute daily predictions over the L3 grid. The final estimates were then obtained

by feeding these intermediate predictions into the XGBoost model. The resulting daily predictions were then averaged over each month to produce the monthly L3 fields.

Care must be taken when applying machine learning algorithms for interpolation. The resulting LST and T_d maps contain predicted values wherever the covariates are available. Ideally, when all covariates are complete, the resulting LST maps should be also spatially continuous. However, certain regions—such as the Alps—lack IASI L2 observations even over a ten-year period. Consequently, the trained models were not exposed to any observations in those complex areas, and their predictions rely solely on data from different environments. In an extreme case, this would be equivalent to training a model on data from the African savannah and attempting to apply it to the Russian boreal forest. To mitigate this issue, L3 LST predictions were discarded in areas with a complete absence of L2 observations.

To illustrate this more clearly, Figure 3.7 shows an example of the LST prediction over the Po Valley for August 2022. The left panel displays the L2 training observations covering the ten-year period (2015–2024), while the right panel shows the spatial domain used for the L3 prediction, where yellow pixels indicate areas where L2 observations are missing across all years, and therefore no predictions were produced. The mask was created by verifying whether at least one L2 observation within the entire period fell within a 0.05° grid cell.

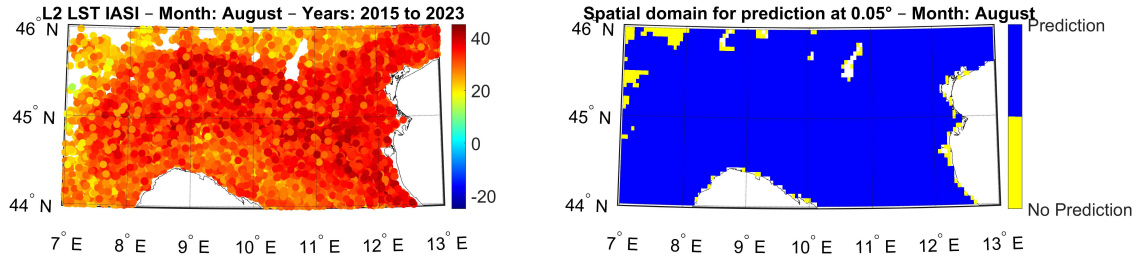


Figure 3.7: Comparison between L2 IASI observations and the derived prediction mask for August 2022. The left panel shows the spatial distribution of L2 observations over the ten-year period, while the right panel shows the spatial domain used for prediction.

The final step consisted of a **residual correction**. As described in [126], residual correction is a post-processing technique that adjusts the final predictions using the residuals, which represent the model errors computed on the training set. Accordingly, an L3 residual map at 0.05° resolution was generated by co-locating the residuals onto the L3 grid, taking into account the corresponding IASI footprints (which vary with the IASI FOV angle). Since L2 observations are spatially scattered, residuals are unavailable across the entire region of interest. To obtain a complete residual field, the thin-plate spline interpolation method (`tpaps` function in Matlab) was applied to fill missing values.

Figure 3.8 illustrates the complete workflow from the IASI LST/ T_d L2 retrieval to the final downscaled L3. Panel (a) represents the IASI L2 retrieval process described in Section 3.1, Panel (b) depicts the training phase discussed in Section 3.2.5, and Panel (c) shows the procedure used to generate the final L3 LST/ T_d maps, as presented in this section.

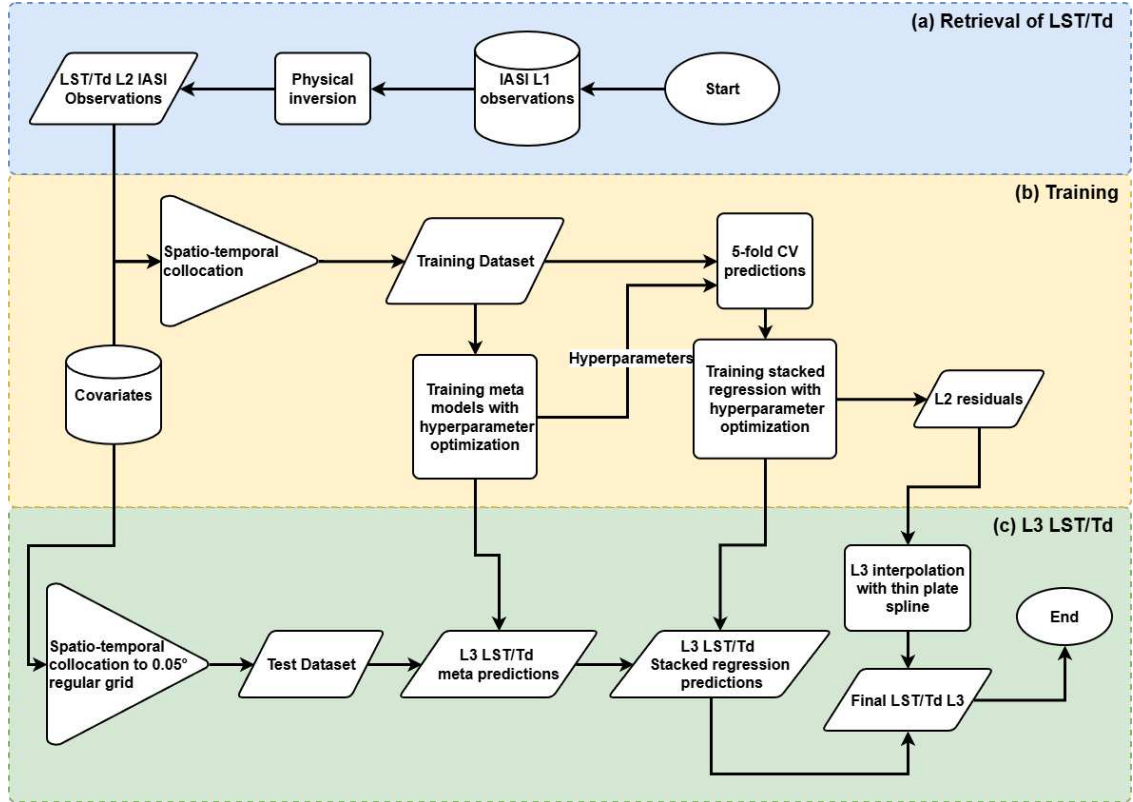


Figure 3.8: Flowchart of the proposed framework. (a) Retrieval of L2 LST/ T_d ; (b) Training; (c) L3 LST/ T_d .



Chapter 4

Results and Discussion

This chapter presents the results of the LST, T_d , and WDI retrieval for the two target regions. The resulting L3 maps are shown, along with their validation and comparison against other reference products. The L3 maps were produced for the entire ten-year period from 2015 to 2024, including both daytime and nighttime overpasses. For the sake of brevity, only the years characterised by the most severe temperature and precipitation anomalies (i.e., drought conditions) have been considered for each area, as identified in the Italian SNPA Climate Report [211].

Specifically, Basilicata and southern Italy experienced the highest temperature anomalies in 2024, followed closely by 2022. In addition, 2024 recorded the second-largest precipitation deficit after 2017, with 2020 ranking third. Therefore, the analysis focused on 2024 for the Basilicata region. In contrast, northern Italy exhibited the opposite pattern: 2024 was the second wettest year since 1961, whereas 2022 recorded the highest temperatures and the lowest precipitation levels on record. The drought that hit northern Italy in 2022 was unprecedented in more than two centuries, and is part of a long-term trend of more frequent and severe drought in the area [166]. For this reason, 2022 was selected for the Po Valley.

To further restrict the analysis, only daytime overpasses were considered, as LST variations during the day are more pronounced. Nighttime temperatures primarily represent the radiative cooling of surfaces, which occurs more uniformly than during the day [114]. Moreover, daytime LST has been shown to play a dominant role in controlling plant phenology [135] and to correlate stronger with NDVI than nighttime LST, making it a more suitable indicator for vegetation water stress monitoring [218].

The trained models for both LST and T_d were first compared in terms of error metrics computed on the L2 observations, in order to highlight the benefits of the Stacked Regression approach. For each region and each month, Mean Squared Error (MAE) and Root Mean Square Error were computed on the cross-validated predictions (see Step 2 of Section 3.2.5). Since the data used for each prediction in each fold differ from those used for training, the resulting MAE and RMSE reflect errors evaluated on independent test sets rather than on the training data, thereby minimizing the risk of choosing an overfitted model.

MAE and RMSE are computed as:

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |\hat{y}_i - y_i|, \quad (4.1a)$$

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N (\hat{y}_i - y_i)^2}, \quad (4.1b)$$

where y_i denotes the IASI L2 observation, $\hat{y}_i$ the L2 cross-validated predictions, and N is the number of L2 pixels.

Then, the daytime L3 maps for LST, T_d , and WDI are presented. The robustness of results for WDI was assessed by validating LST and T_d individually. Section 4.4 and Section 4.5 present the results obtained for the Po Valley and the Basilicata region, respectively.

4.1 Validation of LST

Validating LST products is challenging because only a few ground stations exist worldwide. Given the strong spatial heterogeneity of LST, the focus is on the method's ability to capture finer details and small variations in LST at the target resolution. In this context, the L3 outputs were compared against the L3 LST from MODIS, specifically the MOD11A1 Version 6.1 dataset from NASA <https://lpdaac.usgs.gov/products/mod11a1v061/>. The MODIS LST is a widely used and extensively validated product [234, 145], making it an ideal candidate for comparison. The MODIS sensors, carried on the Terra and Aqua satellites, have provided daily data since 2000 (Terra) and 2002 (Aqua), with a spatial resolution of approximately 1 km at nadir in the TIR channels (31 and 32) used for LST retrieval.

The MOD11 version employed in this study is derived exclusively from the Terra platform, which has acquisition times closest to those of IASI, and is processed using the Generalized Split-Window algorithm [235]. It is well known that in semi-arid and arid areas, there may be significant uncertainty in the estimated emissivities of the MOD11 product, but this should not be the case for the Po Valley region or the Basilicata region. Furthermore, MOD11 tends to be more stable than MOD21, which can exhibit more extreme values, possibly due to incorrect emissivity retrieval or undetected clouds [250]. Only MODIS LST data with good quality and an uncertainty smaller than 2 °C were retained for comparison.

Both IASI and MODIS are sensors onboard polar satellites with a close acquisition time (especially for the Terra satellite). The daily observations were first averaged to monthly composites and then resampled onto the 0.05° grid by averaging all MODIS pixels falling within each 0.05° cell. For each month and year, the following analyses were performed:

- the differences between the two products were computed at both L2 and L3 levels. The IASI L2 observations and the corresponding MODIS LST data were co-located using the procedure described in Section 3.2.4. For each month, the bias (average error) and the

standard deviation were also evaluated. The L2/L3 differences are shown using Kernel Density Estimate (KDE);

- a linear model, $LST_{MODIS} \sim LST_{IASI}$, was fitted to assess the linear relationship. For each month, the coefficient of determination (R^2) was also computed.

4.2 Validation of T_d

T_d validation was carried out using data from the regional Agenzia Regionale per la Protezione dell'Ambiente (ARPA) network, which provides reliable in situ observations across Italy. As T_d is not a direct measure provided by the ARPA networks, T_d was computed using Eq. (3.8) from the air temperature and the relative humidity measured at 2 m. Only stations which provide both variables were considered.

The ARPA stations were spatially and temporally co-located with both IASI L2 and L3 data for the period 2015–2024. For reference, the ERA5 T_d was also included in the analysis. For each month, the average IASI acquisition hour was derived from the corresponding L3 data and used to select the closest hourly records from the ARPA and ERA5 datasets. Then, each ARPA station was spatially matched to the nearest L3 grid cell from both the IASI and the ERA5 datasets. For the L2 data, instead, all IASI L2 observations whose footprints covered the station coordinates were identified. Each L2 observation was then temporally matched with the corresponding ARPA measurement by selecting the closest hourly record. Finally, the paired ARPA measurements and L2 observations were averaged to obtain a representative monthly value for each station. The resulting co-located datasets were then used to compute Pearson correlation, bias, and RMSE between IASI, ERA5, and in situ data.

For the Po Valley, the validation was performed using data from ARPA Emilia and ARPA Lombardia, which provide a significant number of weather stations covering a good portion of the target area. To avoid redundancy due to the high density of ARPA stations in some areas, a spatial filtering was applied using the Density-Based Spatial Clustering of Applications with Noise (DBSCAN) [61] clustering algorithm. DBSCAN is a density-based, non-parametric clustering algorithm which groups together points that are closely packed (points with many nearby neighbours) and marks as outliers points that lie alone in low-density regions. Each station was represented in a three-dimensional space defined by its latitude, longitude, and altitude, and for each identified cluster, the representative station was selected as the one closest to the cluster centroid. In this way, the algorithm ensures a more homogeneous spatial distribution of the stations while preserving elevation variability. Clustering was performed using the MATLAB function `dbscan`, with $\epsilon = 12$ km as the maximum distance for neighbouring stations and `minPts` = 1 as the minimum number of points per cluster. Figure 4.1 shows the ARPA stations for the Po Valley before (top row) and after filtering (bottom row), reducing the total number from 167 to 96. By examining both the mean T_d (2015–2024 average) and

altitude values, we can see that the filtering removed redundant stations located close to each other, while preserving those in more remote or sparsely covered areas. Data were downloaded from <https://dati-simc.arpae.it/opendata/osservati/meteo/storico/> for ARPA Emilia and from <https://www.arpalombardia.it/temi-ambientali/meteo-e-clima/form-richiesta-dati/> for ARPA Lombardia.

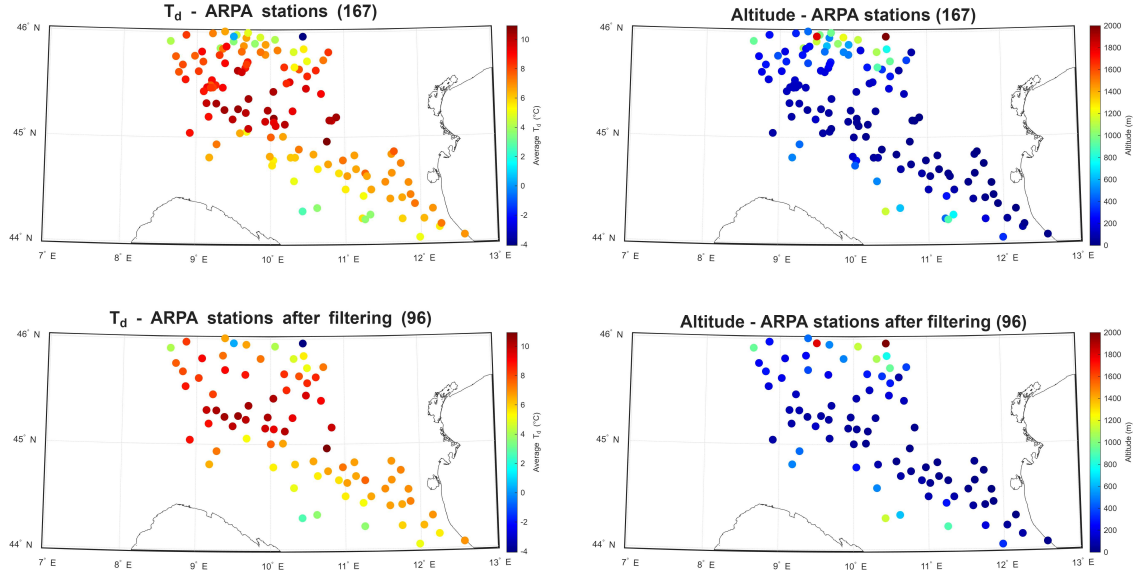


Figure 4.1: ARPA stations used for the Po Valley. The first row shows all available stations, while the second row shows those kept after filtering. In the left column, each station is coloured according to the mean T_d over 2015–2024, and in the right column according to its altitude.

For the Basilicata region, ARPA Basilicata provides a small number of weather stations as shown in Figure 4.2: only six stations provide both air temperature and relative humidity, which are necessary to compute T_d . For this reason, DBSCAN was not applied. Data were downloaded from <https://www.arpab.it/temi-ambientali/aria/qualita-dellaria/monitoraggio-della-qualita-dellaria/qualita-dellaria/dataset/>.

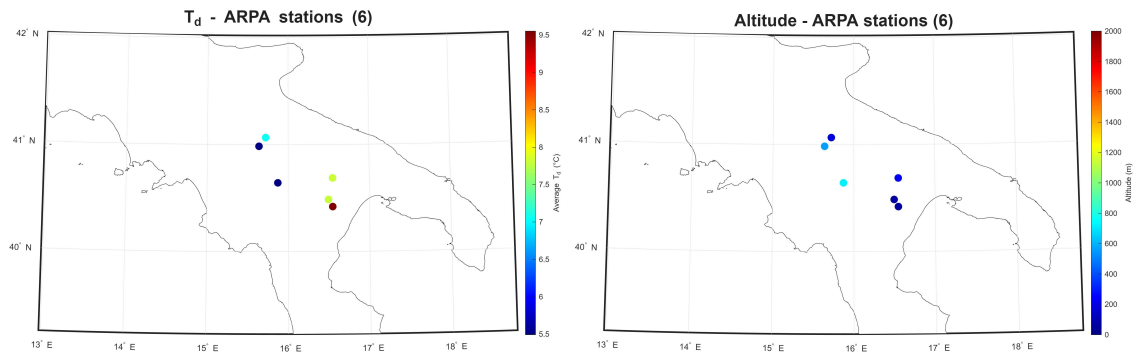


Figure 4.2: ARPA stations used for the Basilicata region. In the left column, each station is coloured according to the mean T_d over 2015–2024, and in the right column according to its altitude.

4.3 Validation of WDI

In the previous section, the validation procedures for LST and T_d retrievals were discussed. As emphasized, the WDI cannot be directly validated. This section therefore complements the previous validation analyses by assessing the ability of the WDI to capture vegetation water stress. To this end, two homogeneous areas have been identified within the two target regions, as described below:

- **Po Valley plains:** latitude 44–45.5°, longitude 8–13°, elevation < 300 m
- **Basilicata:** latitude 39.89–41.14°, longitude 15.33–16.9°

Figure 4.3 presents the selected areas over which the averages were computed.

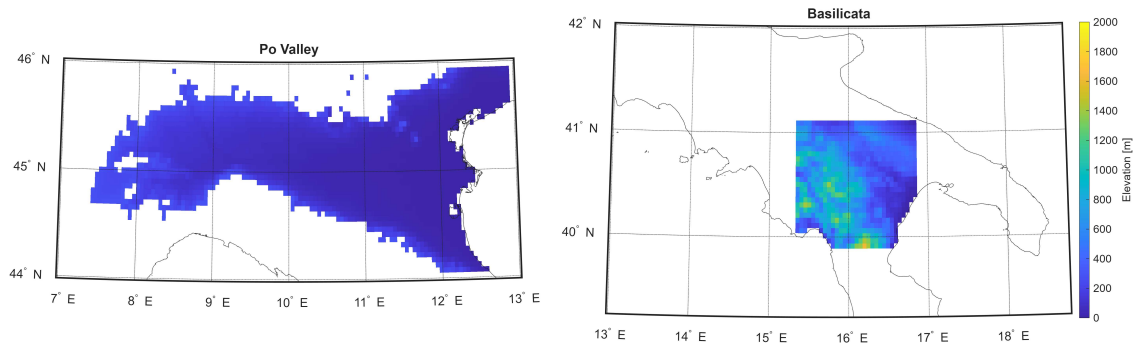


Figure 4.3: Selected geographic areas for WDI analysis. Po Valley plains: latitude 44–45.5°, longitude 8–13°, elevation < 300 m; Basilicata: latitude 39.89–41.14°, longitude 15.33–16.9°, The colour represents the altitude (in meters).

A seasonal average was computed for each year to obtain representative WDI values, highlighting inter-annual differences. Seasons are identified as follows:

- **DJF:** December, January, February
- **MAM:** March, April, May
- **JJA:** June, July, August
- **SON:** September, October, November

These seasonal averages were compared with the literature, using the SNPA report [211]. The most severe stress events identified by the WDI were then compared with other remotely sensed water stress indices, namely the NDMI and Surface Soil Moisture (SSM).

Similarly to the vegetation indices, soil moisture is a parameter highly correlated to air temperature and humidity. Soil moisture is mainly important for two reasons: 1) it is the main water source for agriculture and natural vegetation, and 2) it is a key driver of water and heat fluxes between the ground and the atmosphere, regulating air temperature and humidity. Surface

moisture is negatively related to air temperature [221] and this interaction accounts for about two-thirds of the projected climate change in future climate models [205]. For this reason, the **Surface Soil Moisture (SSM)** is expected to be strongly related to drought and, therefore, was included in the comparison with the WDI. SSM is the relative water content of the top few centimeters of the soil, describing how wet or dry the soil is in its topmost layer, expressed as a percentage of saturation. The Copernicus *1 km SSM Version 1* collection, derived from the Sentinel-1 C-band SAR, was used. The data were downloaded from <https://land.copernicus.eu/en/products/soil-moisture/daily-surface-soil-moisture-v1.0>. The SSM product has a temporal resolution of 1 day and a spatial resolution of 1 km (corresponding to 0.0089°). Observations outside the valid range of 0–100% were filtered out, discarding all the problematic pixels as stated in the Product User Manual (<https://land.copernicus.eu/en/technical-library/product-user-manual-surface-soil-moisture-version-1/@@download/file>).

Plant roots can extend deep into the soil searching for water stored in the lower soil layers. The SSM represents the water content only in the upper soil layer and therefore can be misleading when assessing plant water stress. Conversely, the **Normalized Difference Moisture Index (NDMI)** [28] is generally closer to plant water content and hence was included in the comparison. The NDMI is used to monitor changes in the water content of vegetation canopies and is computed using the normalized difference between the NIR and the SWIR reflectance. The index, firstly proposed by Gao 1996 [28], is defined as:

$$NDMI = \frac{p(0.86\mu m) - p(1.24\mu m)}{p(0.86\mu m) + p(1.24\mu m)} \quad (4.2)$$

Absorption by vegetation liquid water near 0.86 μm is negligible, while a weak liquid water absorption at 1.24 μm is present. As a result, NDMI is sensitive to changes in liquid water content of vegetation canopies. Following [44], the NDMI was evaluated using Sentinel-2 data within the Google Earth Engine (GEE) Python API, based on the B8A and B11 bands. Specifically, the *Harmonized Sentinel-2 MSI: MultiSpectral Instrument, Level-2A* collection available in GEE https://developers.google.com/earth-engine/datasets/catalog/COPERNICUS_S2_SR_HARMONIZED. Since the WDI is a clear-sky product, to ensure a robust comparison it is necessary to remove all cloudy pixels in the NDMI. After a first filtering of tiles with a cloud-cover percentage below 50% (according to the Sentinel-2 metadata), a cloud mask was generated using the `s2cloudless` algorithm [263], available in GEE https://developers.google.com/earth-engine/datasets/catalog/COPERNICUS_S2_CLOUD_PROBABILITY. The `s2cloudless` algorithm uses Light Gradient-Boosting Machine (LightGBM) [84] and generates a product in which each pixel is assigned a cloud probability value. Only pixels with a cloud probability lower than 40% were retained. This threshold was visually chosen to ensure that all clouds were detected, while avoiding the removal of too many valid pixels. Cloud shadows were also removed by projecting shadows from clouds according to the sun's azimuth angle and elevation angles. In addition, a water mask was applied using the CLC 2018 collection available at https://developers.google.com/earth-engine/datasets/catalog/COPERNICUS_CORINE_V20_100m. As a final step, the monthly NDMI

was calculated by merging all tiles of a given month, and the resulting product was then upscaled to a spatial resolution of 1 km.

4.4 Results for the Po Valley

4.4.1 LST

Figures 4.4 and 4.5 present the monthly MAE and RMSE of LST for the Po Valley during daytime and nighttime overpasses, respectively. Among the tested ML algorithms, GBT achieved the best performance, with an MAE of 0.51 °C and an RMSE of 0.70 °C for the daytime overpasses, and an MAE of 0.53 °C and an RMSE of 0.74 °C for the nighttime overpasses. These are already good results, since errors remain below 1 °C. However, combining GBT with the other algorithms through Stacked Regression further improved the performance: MAE and RMSE decreased to 0.48 °C and 0.66 °C for the daytime data, and to 0.51 °C and 0.71 °C for the nighttime data. Although Stacked Regression is computationally more demanding, it further reduced the errors on the L2 observations by approximately 6% for the daytime data and 4% for the nighttime data.

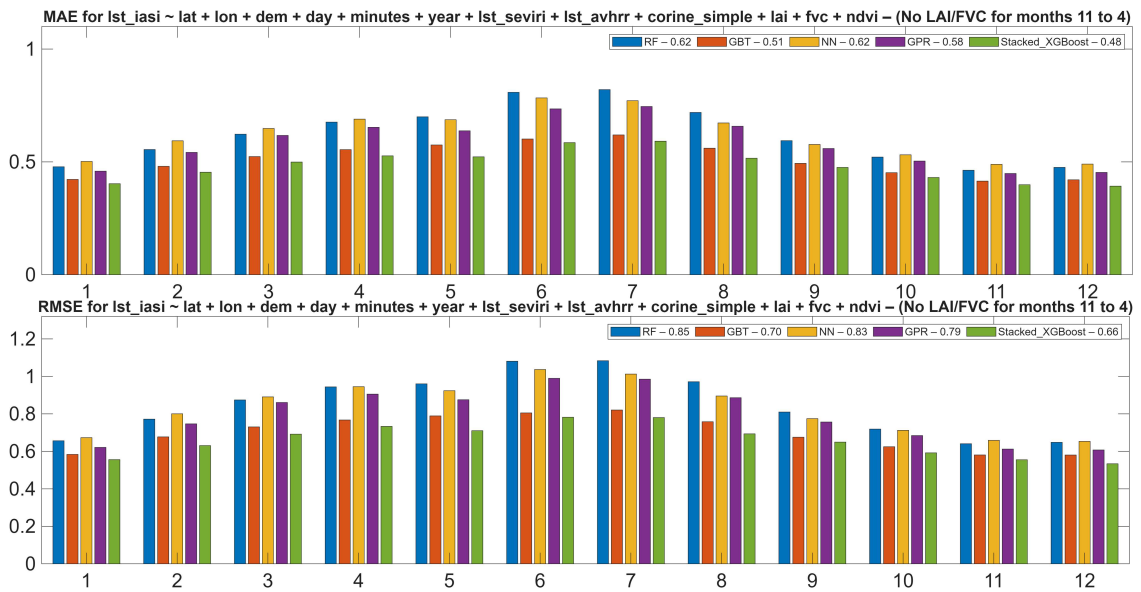


Figure 4.4: Cross-validated MAE (top) and RMSE (bottom) of LST for the tested ML algorithms during daytime overpasses: RF (blue), GBT (orange), NN (yellow), GPR (purple), and Stacked Regression (green). Numbers in the legend represent the average MAE and RMSE across all months.

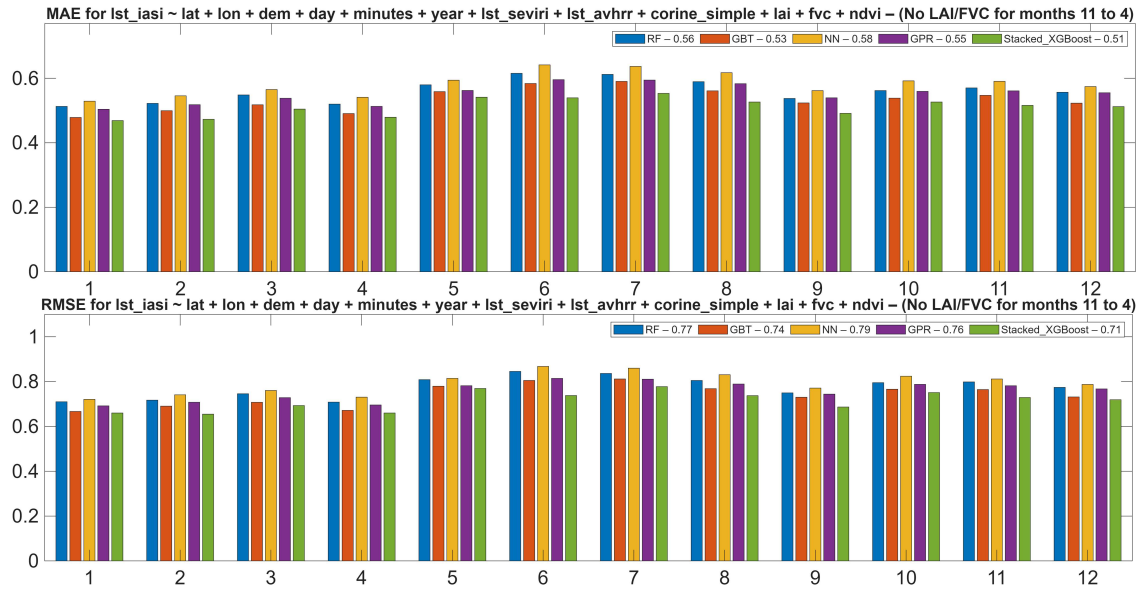


Figure 4.5: Cross-validated MAE (top) and RMSE (bottom) of LST for the tested ML algorithms during nighttime overpasses: RF (blue), GBT (orange), NN (yellow), GPR (purple), and Stacked Regression (green). Numbers in the legend represent the average MAE and RMSE across all months.

Figures 4.6 and 4.7 show the daytime L3 LST maps for 2022 at 0.05° spatial resolution.

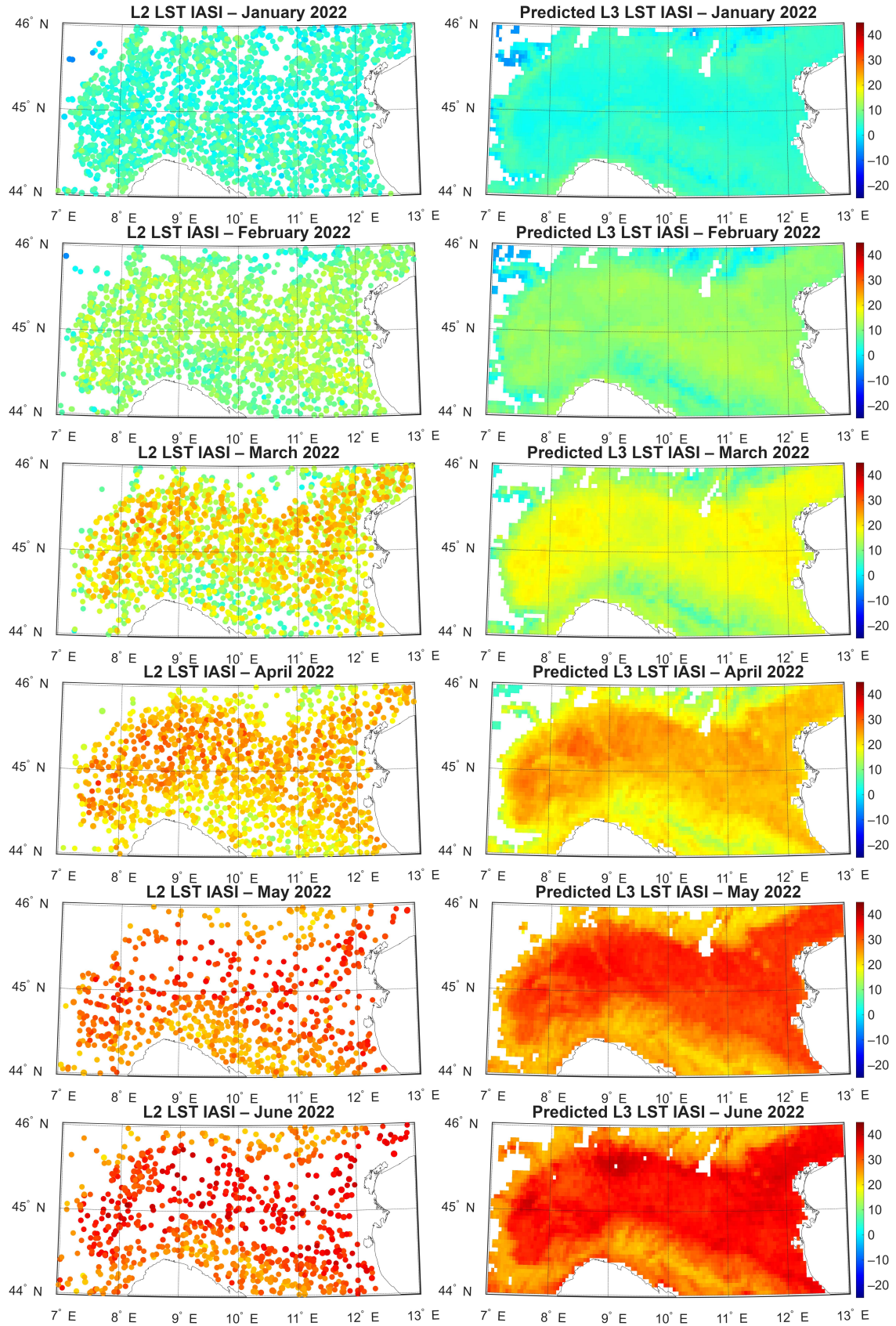


Figure 4.6: Daytime L3 LST maps over the Po Valley for January–June 2022. Left: IASI L2 observations. Right: L3 LST predicted using Stacked Regression; each row represents a month.

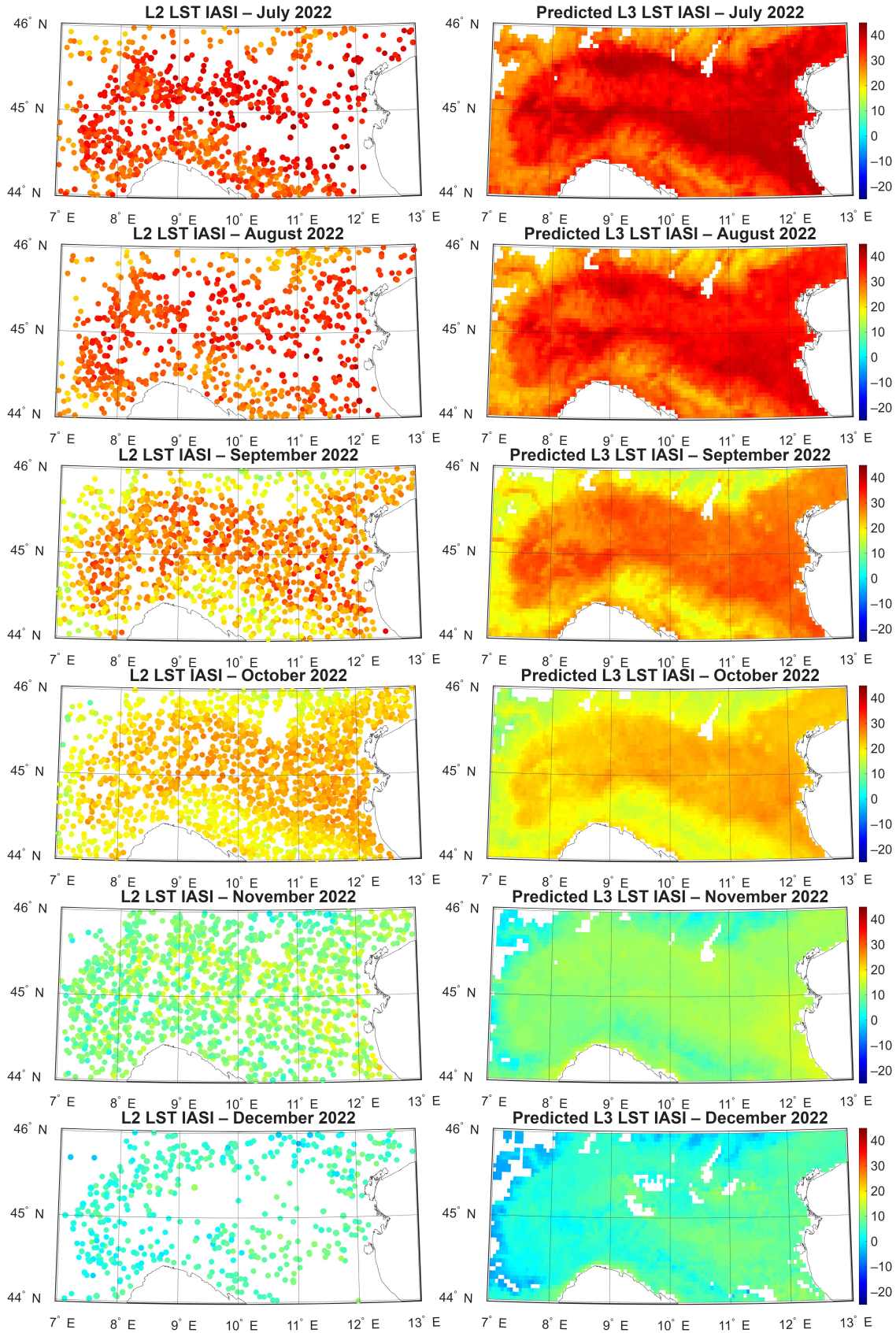


Figure 4.7: Daytime L3 LST maps over the Po Valley for July–December 2022. Left: IASI L2 observations. Right: L3 LST predicted using Stacked Regression; each row represents a month.

There is a strong agreement between the L2 observations and the predicted L3 maps, even though the L2 maps are aggregated products of all L2 observations within a given month (with acquisition times spanning up to 2 h between the first and last observation of a day over our target area). This explains the higher variability in the L2 observations compared to the L3 maps, which, in contrast, represent a monthly product. This is another clear advantage of the proposed methodology: applying a conventional interpolation method, such as kriging, to scattered data that vary both spatially and temporally can produce inaccurate maps. For example, when only a few observations are available in a given area, and these are acquired two hours after the surrounding pixels, the interpolated LST values for that area are likely to be higher than those of the surrounding pixels, resulting in maps that appear “bumpy” or “bubble-shaped”.

A graphical confirmation of the accuracy of the predicted values is the high level of spatial detail visible in the LST maps: based solely on the LST values, we can clearly distinguish the plains, the Apennines, the Alps, and even specific features such as valleys and woodlands. For example, in the area around 8° E and 45° N in April, May, September, and October, the LST has lower values compared to the surrounding areas. Examination of the CLC map reveals that this area, shaped like a horse, corresponds to the Monferrato Hills, a wooded region with elevations between 200 m to 500 m. The lower LST values in this area are explained by the cooling effect provided by healthy vegetation.

Note that this approach is able to retrieve LST even in months with low IASI observation density, thanks to the high-resolution spatial covariates used during the training phase. This can be observed, for example, in May, June, July, August, and particularly in December. Still, it is important to emphasize that in these areas the retrieval is not completely independent from IASI observations since, in the training phase, only spatial areas with IASI coverage were considered (see Section 3.2.6 and Figure 3.7).

A more robust demonstration of the interpolation performance is provided in Figures 4.8 and 4.9, where the IASI L3 outputs were compared against the L3 LST from MODIS. The left column presents the linear differences between the IASI L2/L3 LST values and the MODIS L3 LST, shown using KDE plots, where red represents the L2 errors and blue the L3 errors. Mean and standard deviation values are also reported. The right column shows scatterplots between the predicted IASI L3 LST and the MODIS L3 LST, together with the coefficient of determination (R^2) of the linear fit.

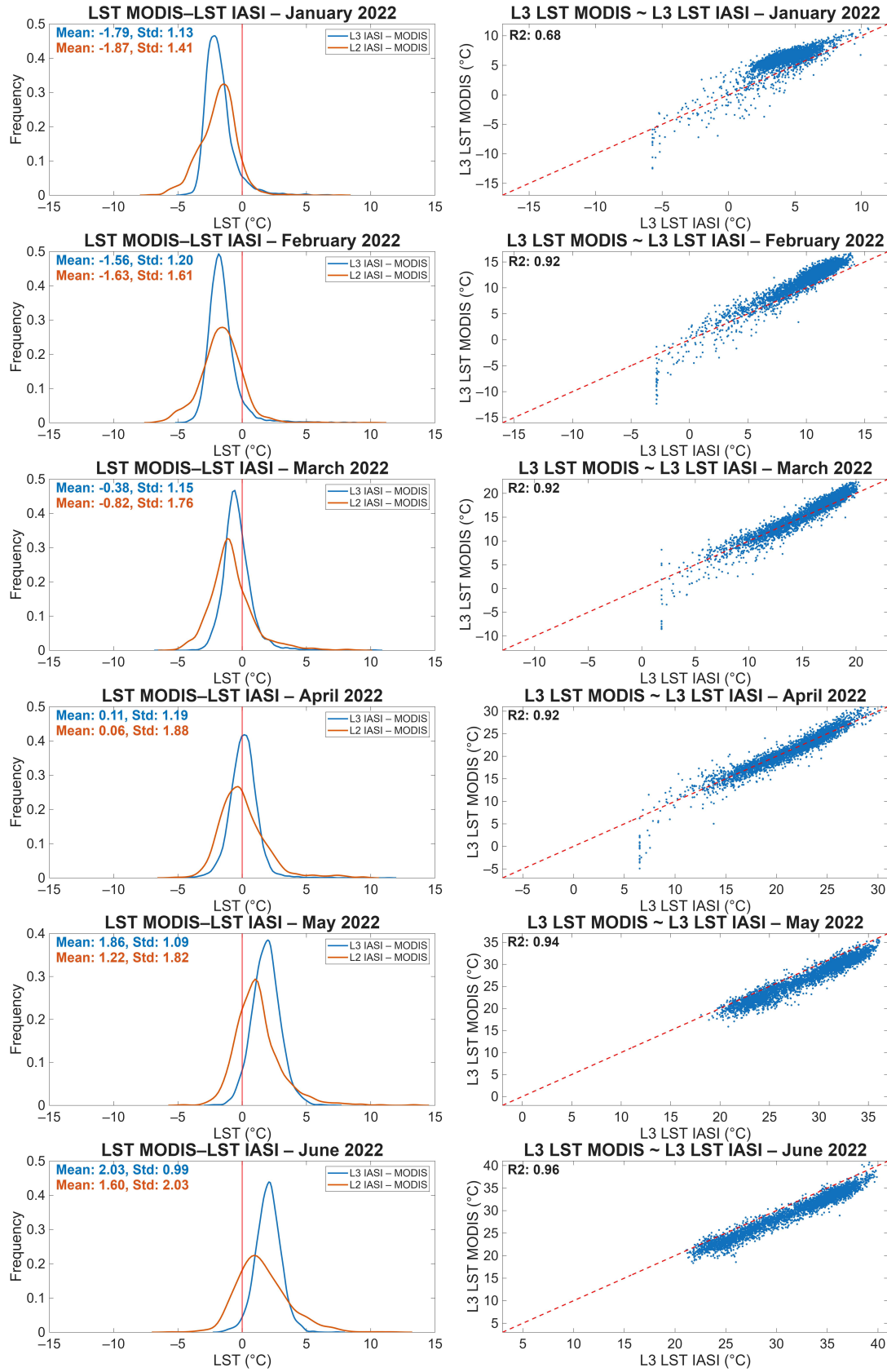


Figure 4.8: Daytime L2/L3 differences (IASI – MODIS) over the Po Valley for January–June 2022. Left: KDE plots of the L2/L3 differences (red and blue), including mean and standard deviation. Right: scatterplots between predicted IASI and MODIS L3 LST values with the coefficient of determination (R^2).

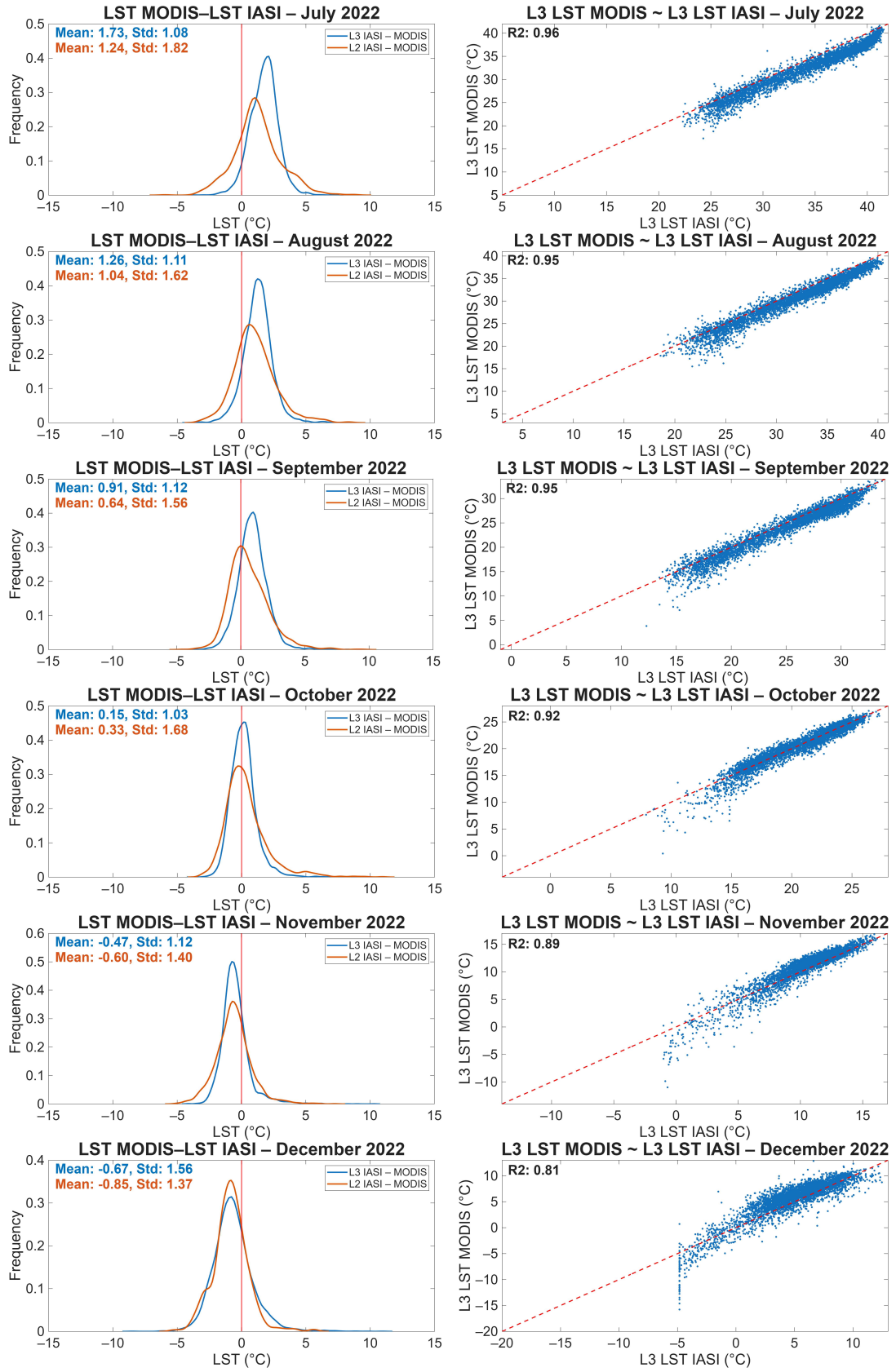


Figure 4.9: Daytime L2/L3 differences (IASI – MODIS) over the Po Valley for July–December 2022. Left: KDE plots of the L2/L3 differences (red and blue), including mean and standard deviation. Right: scatterplots between predicted IASI and MODIS L3 LST values with the coefficient of determination (R^2).

Although the two products were derived from different sensors, with distinct acquisition times and retrieval algorithms, the predicted LST exhibits a strong correlation, with R^2 values greater than 0.90 for almost all months. The standard deviation also shows good results, ranging from 1 °C to 1.5 °C. A portion of these standard deviation values are attributed to the Alps, a region where IASI observations are sparse or entirely absent due to the constant presence of snow. Consequently, the model lacks sufficient training in this area. On the other hand, bias presents a clear seasonal dependence, with positive values during the summer months (indicating higher IASI LST) and negative values in winter (indicating higher MODIS LST). This seasonal bias may be explained by the MODIS SW retrieval algorithm, which uses a fixed emissivity, in contrast to this methodology, which simultaneously retrieves both LST and emissivity. By comparing the IASI L2 LST with the co-located MODIS LST it is also possible to assess the goodness of the downscaling method. The same seasonal bias and a slightly higher standard deviation persists, indicating that the differences arise from the products themselves rather than our downscaling method, which, by contrast, slightly reduced the differences.

The seasonal variability found with MODIS was also addressed by comparing the co-located L2 LSTs from IASI, AVHRR, SEVIRI, and MODIS. Figures 4.10 and 4.11 present the KDE plots and boxplots of the differences between the L2 LST. The first column displays the L2 differences using KDE plots, including the mean and standard deviation: blue curves represent the L2 differences between IASI and AVHRR, red curves represent those between IASI and SEVIRI, and yellow curves represent those between IASI and MODIS. The second column shows the same differences using boxplots, with the corresponding R^2 coefficients indicated on the x -axis.

Among the different LST products, the one derived from AVHRR shows the highest agreement with IASI, exhibiting the highest R^2 values (with the only exception of January), the lowest absolute bias (generally lower than 1 °C) without an evident seasonal pattern, and with a standard deviation lower than <1.67 °C. This is predictable, as both sensors are onboard the same platform. In contrast, MODIS and SEVIRI have biases that vary significantly throughout the year, with a very negative bias during winter months and a positive bias in the summer months, consistent with the patterns observed for the L3 product in Figures 4.8 and 4.9. Additionally, their standard deviation values are higher than those of AVHRR but do not show any seasonal patterns. SEVIRI presents higher R^2 values compared to MODIS, similar to those of AVHRR.

However, due to the strong spatial and temporal variability of LST, comparing IASI and MODIS data acquired with a time difference of one hour or more can lead to temperature differences of several degrees in certain regions. It is also important to note that, in order to maintain a sufficient number of data points for comparison, we considered MODIS, AVHRR, and SEVIRI pixels with LST uncertainties up to 2 °C (nominal quality), as described in Section 3.2.2. Furthermore, this temporal difference influences not only the LST values due to the diurnal temperature cycle, but also the number of pixels averaged within each IASI footprint, which depends on cloud cover. For example, let us consider an IASI observation acquired at a specific time under clear-sky conditions. Since LST products from other sensors (e.g., MODIS) have a much finer spatial resolution, multiple observations fall within the IASI footprint. If the sky remains completely

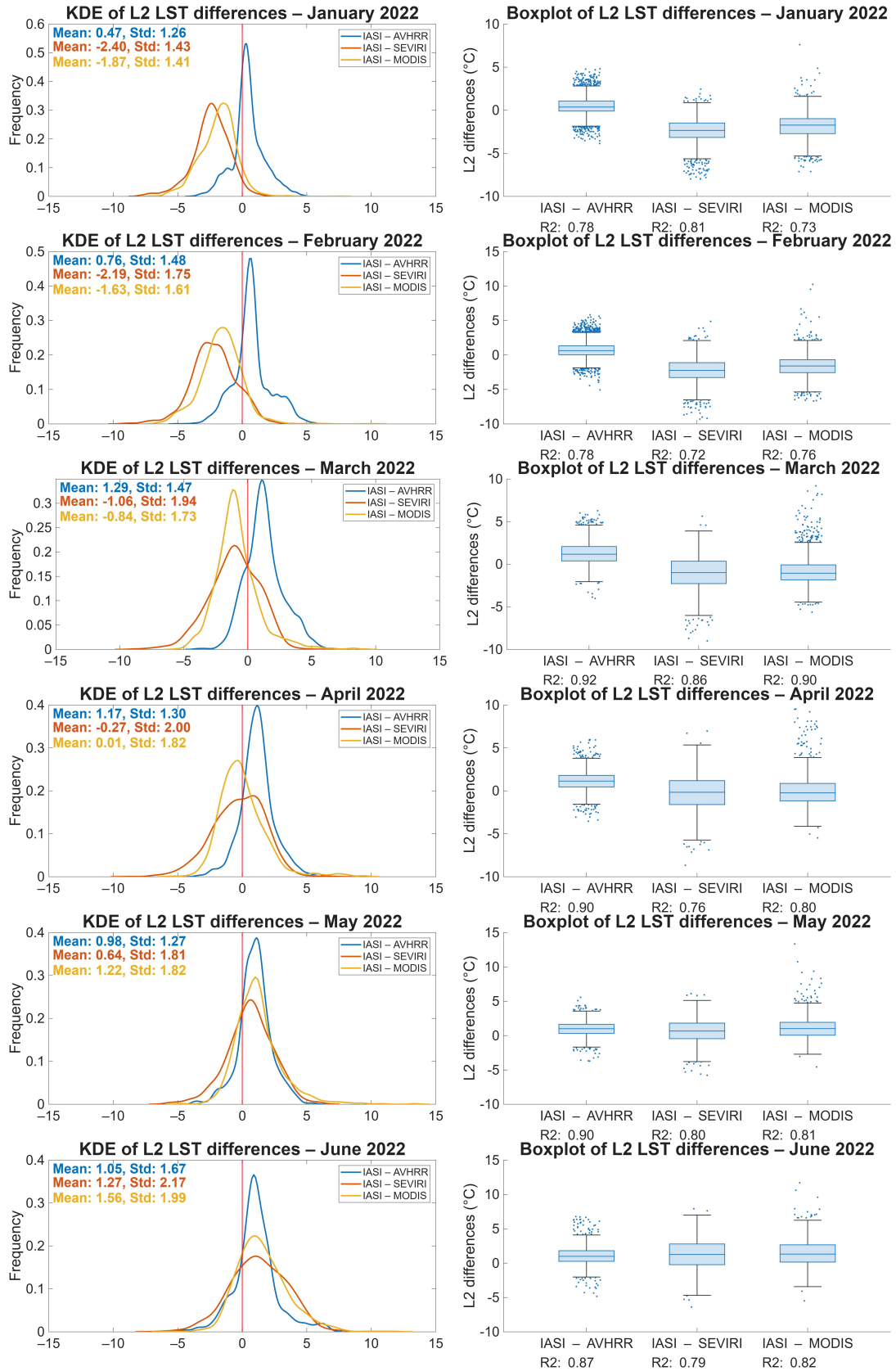


Figure 4.10: Daytime comparison of LST from IASI, AVHRR, SEVIRI, and MODIS for January–June 2022. Left: KDE plots of L2 differences (blue: AVHRR, red: SEVIRI, yellow: MODIS), including mean and standard deviation. Right: boxplots of the same differences with corresponding R^2 values on the x -axis.

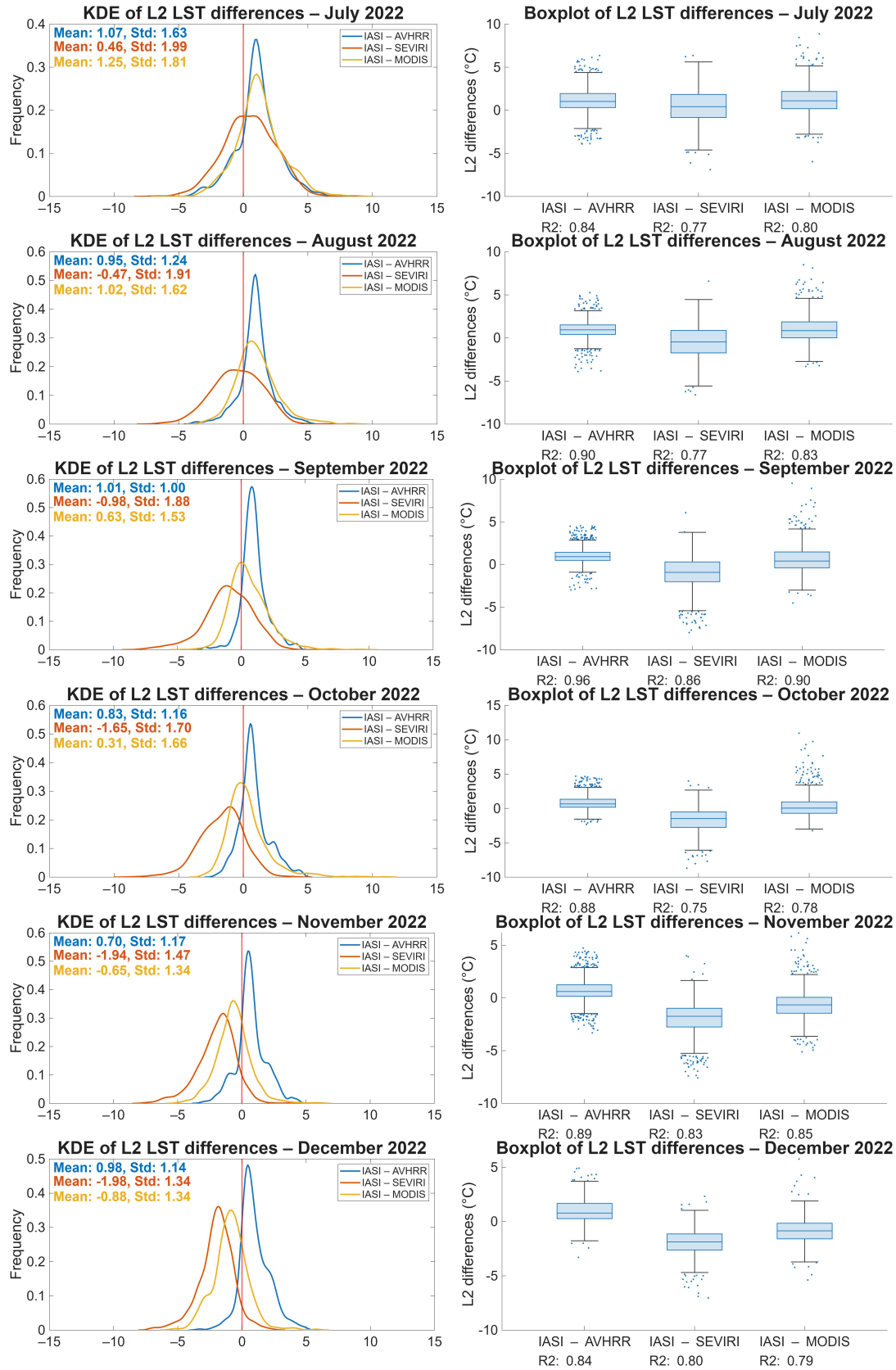


Figure 4.11: Daytime comparison of LST from IASI, AVHRR, SEVIRI, and MODIS for July–December 2022. Left: KDE plots of L2 differences (blue: AVHRR, red: SEVIRI, yellow: MODIS), including mean and standard deviation. Right: boxplots of the same differences with corresponding R^2 values on the x -axis.

cloud-free, we will average always the same number of MODIS observations; hence the two sensors observe essentially the same scene spatially, though at different resolutions and acquisition times. This means that, after spatial co-registration (i.e. averaging MODIS observations within the IASI footprint) and temporal alignment, the differences between the two products mainly reflect sensor characteristics and retrieval algorithms rather than sampling or representativeness effects.

However, within the time window between the IASI observation and the corresponding LST observations from another sensor, clouds may move and partially cover the footprint. In effect, cloud coverage and the same land coverage can affect the comparison among different sensors because the other platforms overpass the given area at various times, and cloud dynamics are much faster than the delay among the platforms themselves. This explains why these results show better agreement with AVHRR, a companion instrument of IASI onboard the same MetOp satellites.

Cloud evolution can reduce the number of clear-sky observations used in the averaging process, resulting in LST values that represent only a portion of the footprint. This could explain the seasonal bias observed with SEVIRI and MODIS: during winter months, clouds are much more prevalent, reducing the number of LST observations averaged for each IASI footprint. To substantiate this claim, AVHRR, which shares the same platform and observes the exact same scene, does not show this seasonal bias. Despite that, we observe a strong correlation between the two L3 products, with R^2 values reaching up to 0.95 in some months. The L2 comparisons among the four LST datasets also reveal a strong correlation, with AVHRR showing the highest R^2 , followed by SEVIRI and MODIS. However, the R^2 values are still the highest in the L3 comparison.

4.4.2 T_d

Figures 4.12 and 4.13 present the monthly MAE and RMSE of T_d for the Po Valley during daytime and nighttime overpasses, respectively. Also for T_d , GBT achieved the best performance among

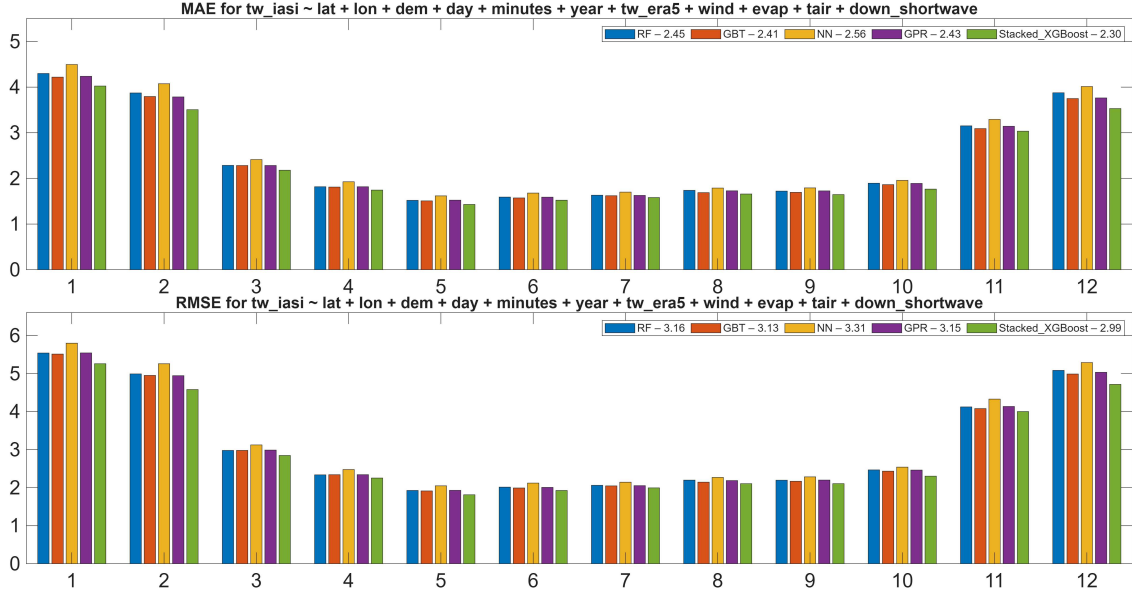


Figure 4.12: Cross-validated MAE (top) and RMSE (bottom) of T_d for the tested ML algorithms during daytime overpasses: RF (blue), GBT (orange), NN (yellow), GPR (purple), and Stacked Regression (green). Numbers in the legend represent the average MAE and RMSE across all months.

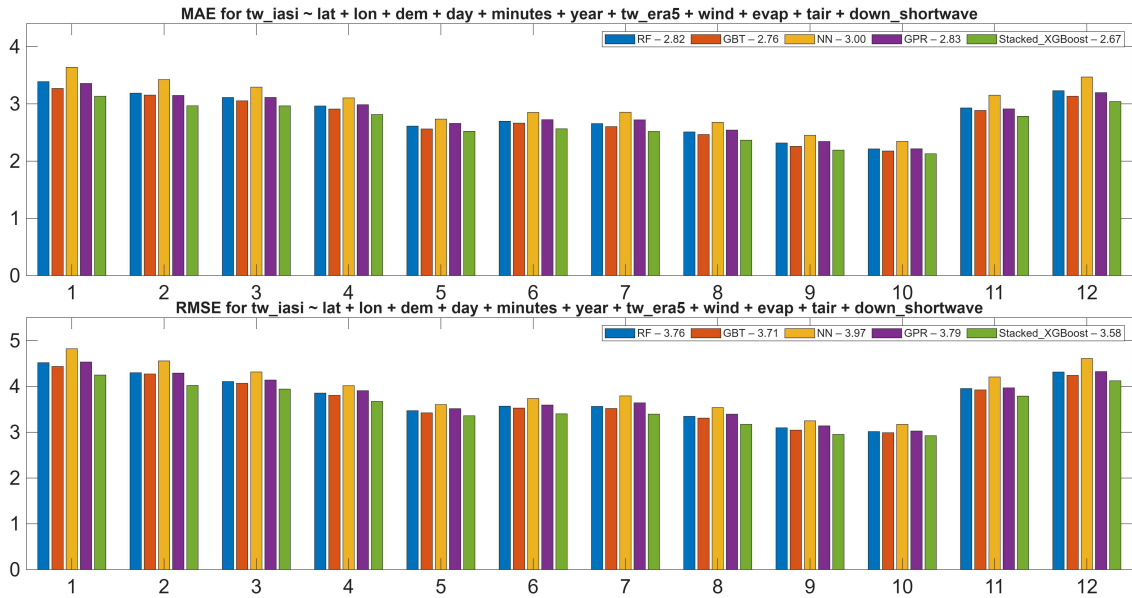


Figure 4.13: Cross-validated MAE (top) and RMSE (bottom) of T_d for the tested ML algorithms during nighttime overpasses: RF (blue), GBT (orange), NN (yellow), GPR (purple), and Stacked Regression (green). Numbers in the legend represent the average MAE and RMSE across all months.

the tested ML algorithms, with an MAE of 2.41 °C and an RMSE of 3.13 °C for the daytime overpasses, and an MAE of 2.76 °C and an RMSE of 3.71 °C for the nighttime overpasses. Again, Stacked Regression further improved the performance: MAE and RMSE decreased to 2.30 °C and 2.99 °C for the daytime data, and to 2.67 °C and 3.58 °C for the nighttime data, with an improvement of 4.5% for the daytime data and 3.5% for the nighttime data. Compared with LST, training on T_d is more challenging:

- The ERA5-Land predictors used in the model have approximately the same spatial resolution as IASI, and therefore do not provide additional high-resolution spatial information.
- A temporal mismatch exists, since ERA5-Land data are available hourly, whereas SEVIRI provides observations every 15 minutes (with a maximum difference of 7.5 minutes) and AVHRR is on the same platform as IASI, providing near-synchronous acquisition.
- While LST from SEVIRI, AVHRR, and IASI all represent radiometric skin temperatures retrieved in a similar way, the ERA5-Land T_d is a reanalysis product that combines a NWP model with data assimilation from diverse observations.
- There is also a sampling bias since TIR LST is clear-sky only, while T_d from reanalysis is all-sky and model-assisted.

These factors explain the higher MAE and RMSE values obtained for T_d compared with LST. Similarly to LST, daytime L3 T_d maps for 2022 were generated at a spatial resolution of 0.05° (Figures 4.14 and 4.15).

The L3 T_d maps appear much smoother than those of LST, with smaller variations both across the months and spatially. This is, however, not necessarily an issue, since LST typically shows larger variations over short distances than T_d , which, by contrast, is generally smoother at the mesoscale because of near-surface atmospheric mixing. Indeed, the validation of T_d with ARPA data confirms the high consistency of the interpolated product. For the Po Valley, 96 ARPA stations were used in the validation step. To simplify, Figure 4.16 shows daytime time-series plots of T_d from ARPA (blue), IASI (red), and ERA5 (green) for four representative stations, together with their corresponding Pearson correlation coefficients. This visualization helps to assess how the different datasets behave over time. The correlations among the three T_d products are very high, with values close to 1 and minor differences between IASI and ERA5, showing slightly better agreement for ERA5.

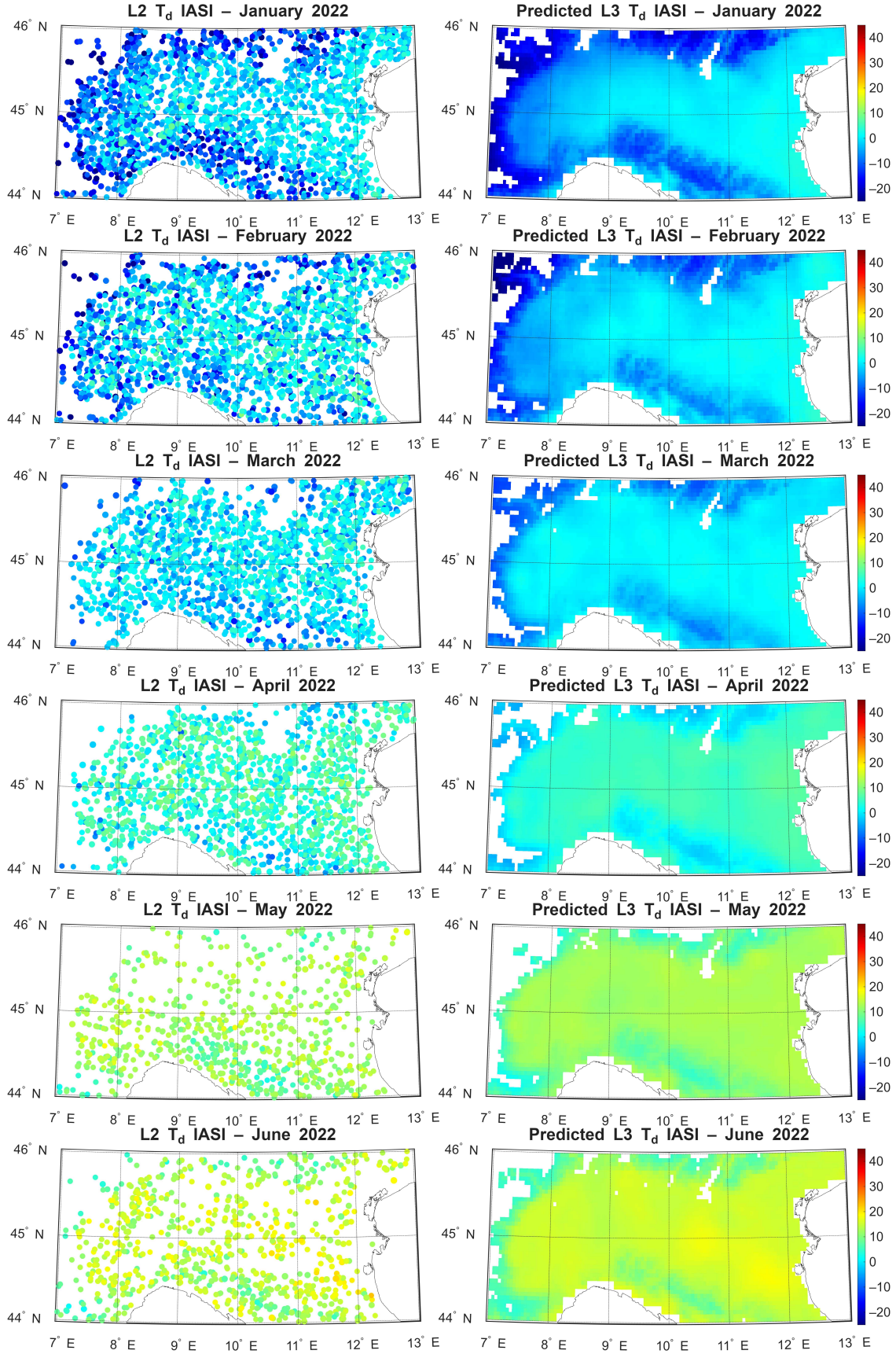


Figure 4.14: Daytime L3 T_d maps over the Po Valley for January–June 2022. Left: IASI L2 observations. Right: L3 T_d predicted using Stacked Regression; each row represents a month.

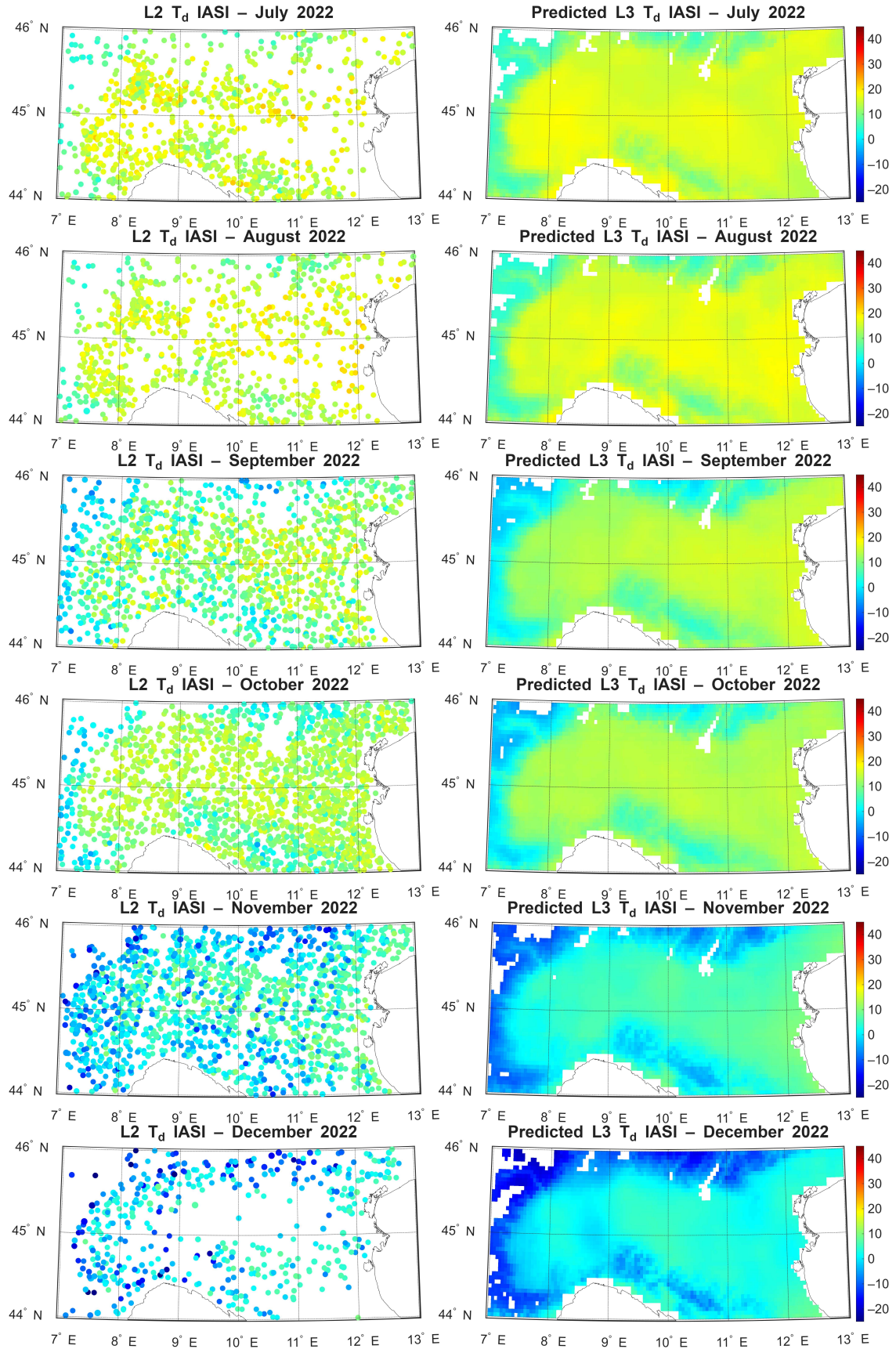


Figure 4.15: Daytime L3 T_d maps over the Po Valley for July–December 2022. Left: IASI L2 observations. Right: L3 T_d predicted using Stacked Regression; each row represents a month.

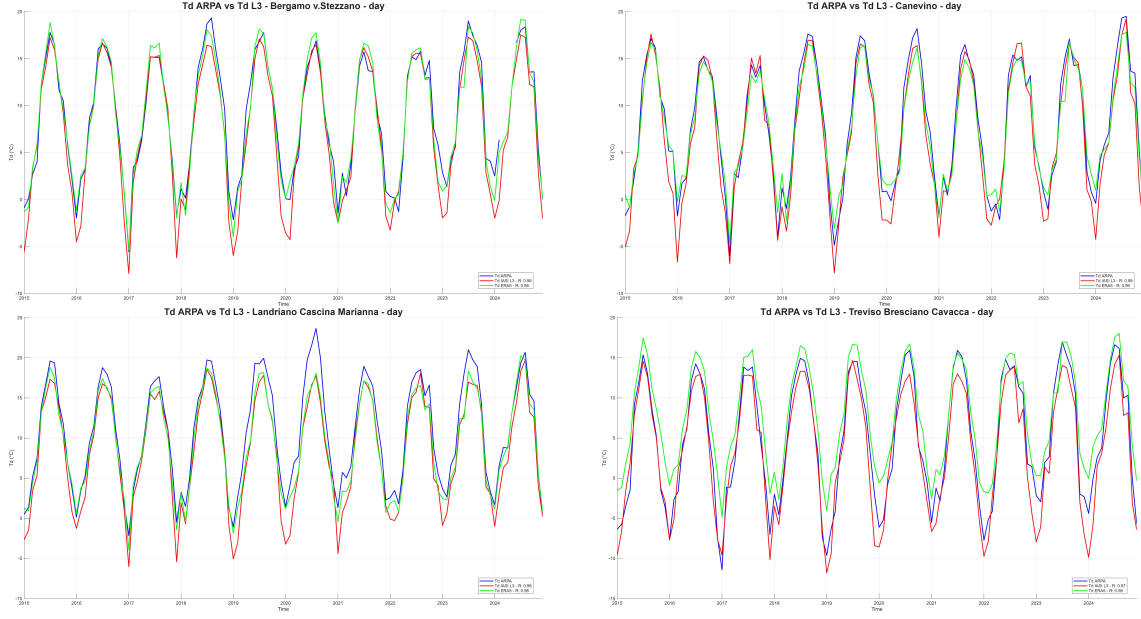


Figure 4.16: Daytime T_d time-series from ARPA (blue), IASI (red), and ERA5 (green) for four representative stations in the Po Valley.

To confirm that these results are consistent across the entire region, Figure 4.17 shows the validation of T_d using all 96 ARPA stations. The validation is performed for both daytime (first row) and nighttime overpasses (second row). ARPA T_d is compared with IASI L3 T_d (first column), ERA5 T_d (second column), and IASI L2 T_d (third column). For each comparison, the Pearson correlation coefficient, bias, and RMSE were computed.

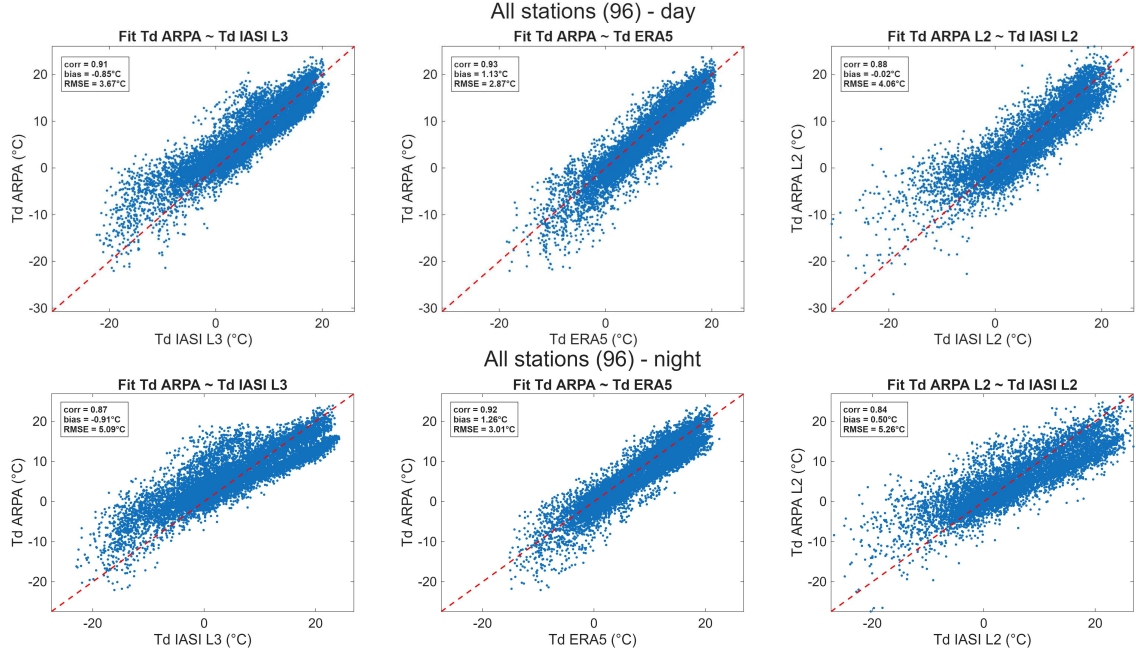


Figure 4.17: Validation of T_d using all 96 ARPA stations over the Po Valley. The first and second rows correspond to daytime and nighttime overpasses, respectively. Columns show the comparison of ARPA T_d with IASI L3 (left), ERA5 (centre), and IASI L2 (right). Pearson correlation, bias, and RMSE are reported for each case.

First, the downscaled IASI T_d shows a very high agreement with ARPA stations, with correlation coefficients of 0.91 for daytime and 0.87 for nighttime. These results are very close to those obtained between ERA5 and ARPA ($r = 0.93$ and $r = 0.92$, respectively). The bias analysis also indicates good performance, with absolute values below 1°C for IASI L3, slightly better than ERA5, although the two T_d datasets exhibit opposite bias signs: negative for IASI and positive for ERA5. Conversely, the RMSE is higher for IASI. However, it must be noted that ERA5 is a reanalysis product that also assimilates ground-based observations, and therefore it is expected to perform better than a fully satellite-based product.

Moreover, the comparison between IASI L2 and L3 T_d shows that, although the interpolation introduced a small bias, it actually increased the correlation and reduced the RMSE. Lastly, it must be remembered that ground-based measurements represent point observations, whereas satellite-derived values represent areas spanning several kilometers. Increasing spatial resolution is a way to bring satellite-derived estimates closer to in-situ measurements.

4.4.3 WDI

Figure 4.18 shows the daytime L3 WDI maps for 2022 at a spatial resolution of 0.05° . From the maps, it is clear that T_d provides complementary information to the LST, as the resulting WDI reveals patterns that are not visible in the LST and T_d alone. For example, in January the Po Valley plains exhibit very low WDI values ($WDI < 5^\circ\text{C}$), whereas the Apennines and, in particular, the Alps show values exceeding 20°C . Due to the orographic conformation, air in the Po Valley tends to stagnate, resulting in low temperatures and high humidity, which explains WDI values close to zero; in this region, frost, fog, and dew are very common. Conversely, at high altitudes temperatures decrease, but humidity also drops, leading to even lower T_d and consequently very high WDI values. Further evidence of the index's ability to distinguish between dry and humid conditions is provided by the area around 8.3°E and 45.3°N , corresponding to the Vercelli-Novara plain. This region is extensively cultivated with rice fields, which are often still flooded, resulting in consistently high local humidity and a moderating effect on temperature extremes. These conditions are well captured by the WDI, which shows substantially lower values compared to the surrounding areas.

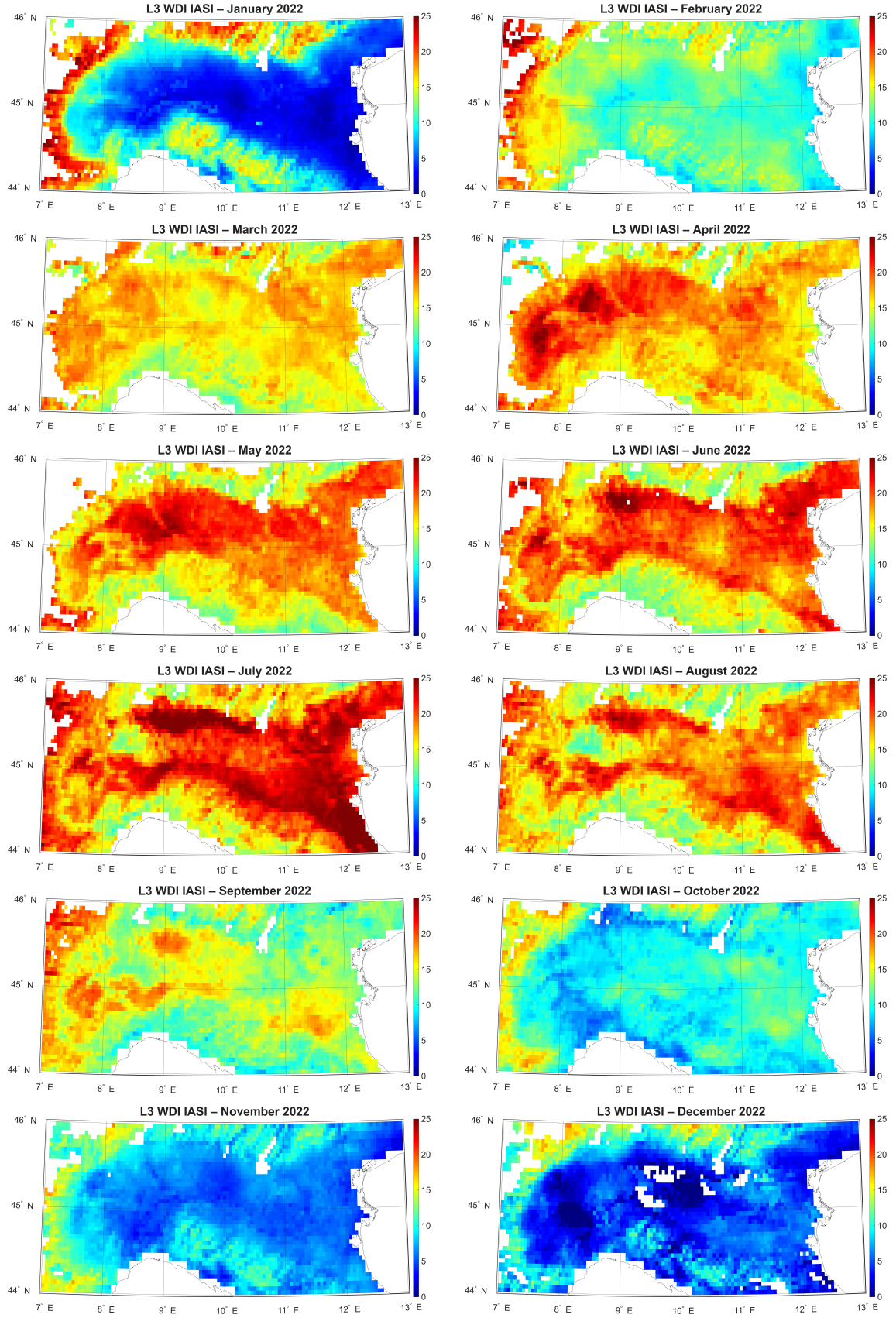


Figure 4.18: Daytime L3 WDI maps over the Po Valley for 2022 computed as the difference between the IASI L3 LST and T_d .

To identify the years with the highest water stress, Figure 4.19 shows the seasonal distribution of WDI values for each year, restricting the analysis to the areas depicted in Figure 4.3. Two years show exceptionally high WDI values: 2017 and 2022. This is fully consistent with the literature, as both years, especially 2022, recorded the highest temperatures and lowest precipitation levels on record. Interestingly, 2024 exhibits relatively low WDI values. Although 2024 in the SNPA report ranked third in terms of positive temperature anomalies (with 2022 being the first, followed by 2023), precipitation levels were the second highest ever recorded since 1961, explaining the low WDI values. Overall, the WDI not only successfully captured the years associated with water deficit, but also distinguished between years that were both hot and dry and those that were only hot or only dry.

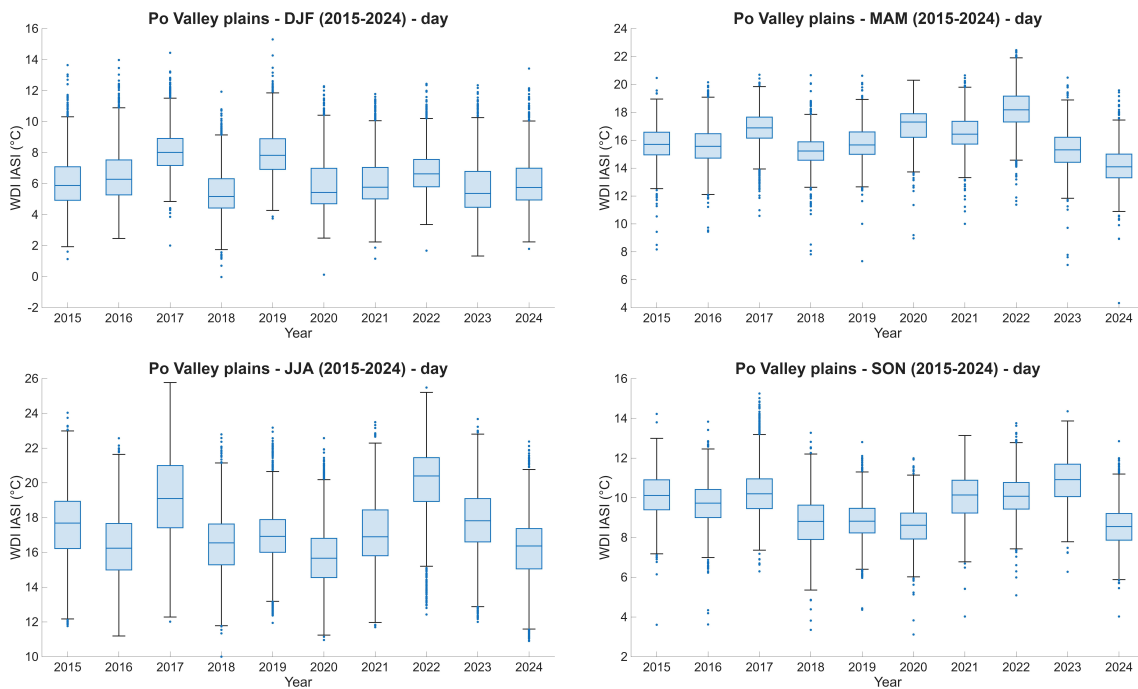


Figure 4.19: Daytime seasonal WDI boxplots over the Po Valley by year. Each boxplot represents the distribution of WDI values selected according to the defined criteria within the Po Valley.

A further confirmation of the WDI's ability to detect water deficit conditions is provided by its comparison with SSM and NDMI. The comparison was restricted to two representative cases: April and May 2023 (Figure 4.20), and June 2022 and 2024 (Figure 4.21).

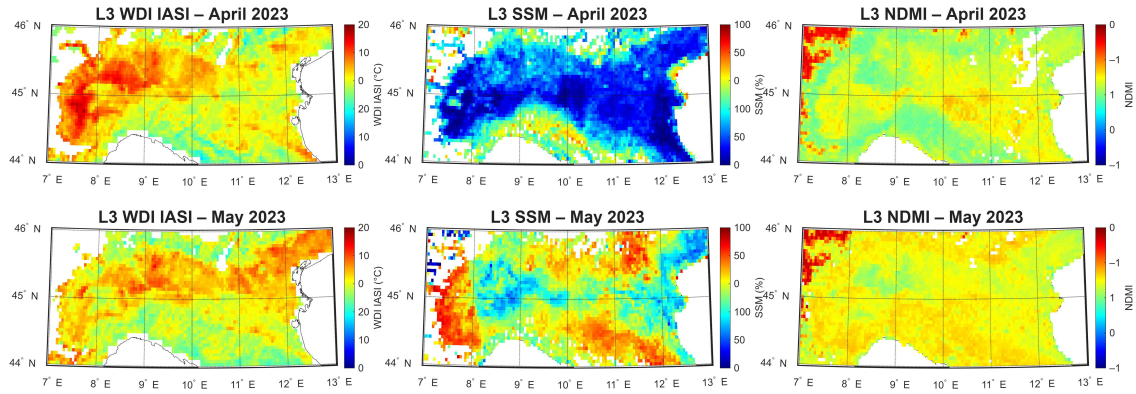


Figure 4.20: Comparison between daytime WDI, SSM and NDMI for April (top) and May (bottom) 2023 over the Po Valley.

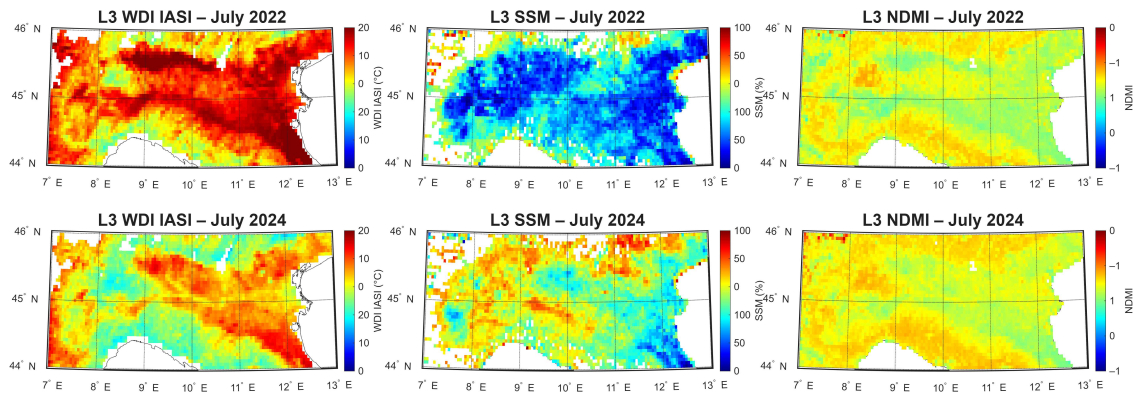


Figure 4.21: Comparison between daytime WDI, SSM and NDMI for June 2022 (top) and June 2024 (bottom) over the Po Valley.

From a first analysis, the SSM appears to be the index most consistent with the WDI: when SSM is low WDI is generally higher. May 2023 was hotter than April, and thus a higher WDI should be expected. However, the opposite occurred, with April showing the highest WDI values. Indeed, by looking at the SSM, we can clearly see that in April the soil was almost completely dry while in May it was significantly wetter. This observation is in agreement with both [26] and [58], which identified a precipitation deficit in the first four months of the year followed by an exceptionally wet May (some regions recorded precipitation two times above the reference period 1991–2023). Conversely, June 2022 and 2024 were both characterised by very high temperatures but totally different precipitation levels. From the SSM, it is clear that June 2024 was much wetter than 2022, as also reported in the SNPA report [211]. Unsurprisingly, the WDI exhibits the same trend but in the opposite direction, with clearly higher values in 2022 and lower in 2024. This further confirms the link between the WDI and soil moisture.

NDMI also shows a similar relationship with the WDI: high NDMI values, which indicate healthy vegetation without water stress, correspond to low WDI values. For example, in Figure 4.20, NDMI shows higher values in May 2023 but lower in April 2023. The WDI displays the opposite pattern, confirming its ability to capture vegetation water deficit. Although this rela-

tionship might be partially masked by the vegetation growth peak in May, the same trend is also observed in Figure 4.21, where by looking at the same month, seasonal vegetation effects should be minimal. As before, the higher WDI observed in 2022 corresponds to lower NDMI values, while in 2024 the situation is reversed, with lower WDI and higher NDMI values, consistent with the abundant precipitation reported that year (also highlighted by the SSM).

4.5 Results for the Basilicata

4.5.1 LST

Figures 4.22 and 4.23 present the monthly MAE and RMSE of LST for the Basilicata region during daytime and nighttime overpasses, respectively. Among the tested ML algorithms, GBT also achieved the best performance for this region, with an MAE of 0.60°C and an RMSE of 0.81°C for the daytime overpasses, and an MAE of 0.57°C and an RMSE of 0.77°C for the nighttime overpasses. Again, these are already good results, as the errors remain well below 1°C , although slightly higher than those obtained for the Po Valley. However, combining GBT with the other algorithms through Stacked Regression further improved the performance: MAE and RMSE decreased to 0.55°C and 0.74°C for the daytime data, and to 0.54°C and 0.73°C for the nighttime data. Compared to GBT, Stacked Regression further reduced the errors by approximately 8% for the daytime data and 5% for the nighttime data, representing a slightly greater improvement than that obtained for the Po Valley.

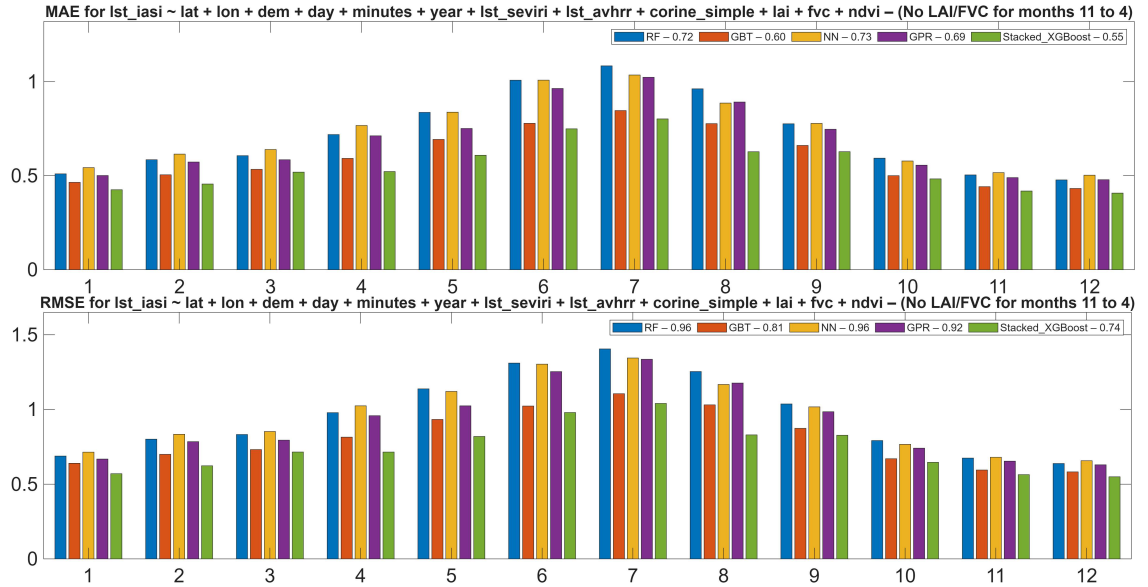


Figure 4.22: Cross-validated MAE (top) and RMSE (bottom) of LST for the tested ML algorithms during daytime overpasses: RF (blue), GBT (orange), NN (yellow), GPR (purple), and Stacked Regression (green). Numbers in the legend represent the average MAE and RMSE across all months.

Figures 4.24 and 4.25 show the L3 LST maps at a spatial resolution of 0.05° . There is a strong agreement between the L2 observations and the predicted L3 maps. Based solely on the LST values, it is possible to clearly distinguish the plains from the mountains, as well as a positive west–east gradient. This gradient is related to land-cover differences, as also depicted by the CLC shown in Figure 3.3, where the Tyrrhenian side is covered by broadleaf forests, while the eastern side, toward Puglia, is dominated by olive groves and agricultural land.

It is interesting to note that during the summer months (June, July, and August) there is a shortage of L2 observations along the Apennine chain and in the Puglia region. This behaviour

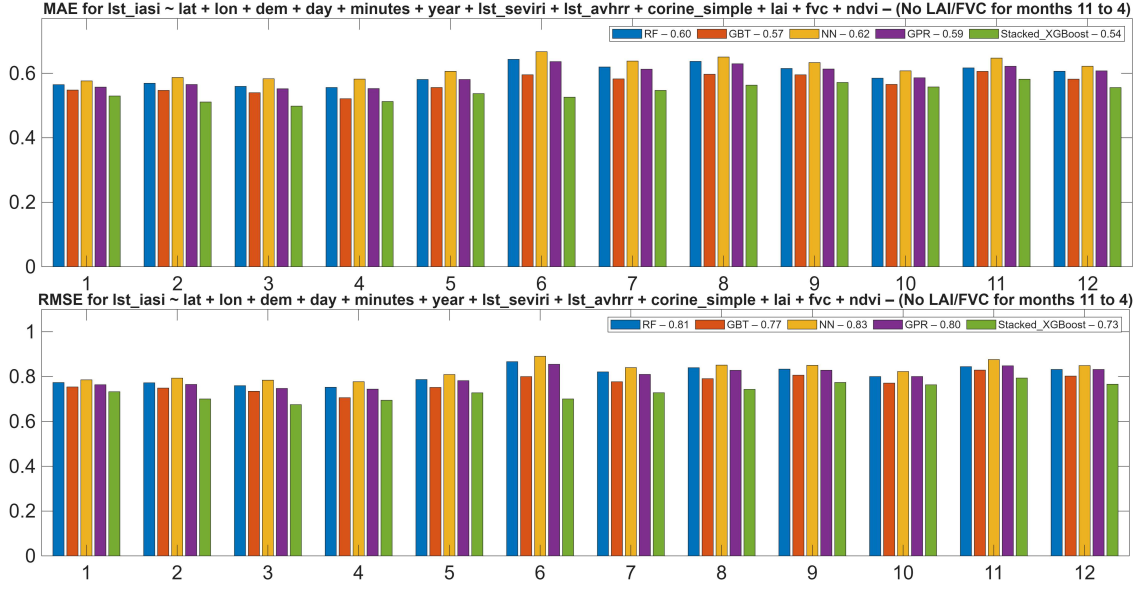


Figure 4.23: Cross-validated MAE (top) and RMSE (bottom) of LST for the tested ML algorithms during nighttime overpasses: RF (blue), GBT (orange), NN (yellow), GPR (purple), and Stacked Regression (green). Numbers in the legend represent the average MAE and RMSE across all months.

also occurs in other years, although fortunately not every year, suggesting that convective clouds or haze develop in the morning and are captured by the AVHRR sensor (IASI cloudy pixels are discarded based on the internal AVHRR cloud mask). This interpretation is further supported by the nighttime images, which, in contrast, show a much larger number of valid pixels, as shown in Figure 4.26.

Figures 4.27 and 4.28 show the comparison between the IASI L3 outputs and the L3 LST from MODIS. The left column presents the linear differences between the IASI L2/L3 LST values and the MODIS L3 LST, shown using KDE plots, where red represents the L2 errors and blue the L3 errors. Mean and standard deviation values are also reported. The right column shows scatterplots between the predicted IASI L3 LST and the MODIS L3 LST, together with the coefficient of determination (R^2) of the linear fit.

The predicted LST exhibits a strong correlation for this region, with R^2 values greater than 0.90 for most months. The standard deviation also remains low, with values below 1.5°C , with July being the only exception. The standard deviation for Basilicata is generally lower than that for the Po Valley, except in the summer months. The bias is also different, since it is generally positive and shows a less evident seasonal pattern.

The seasonal variability found with MODIS was also addressed by comparing the co-located L2 LSTs from IASI, AVHRR, SEVIRI, and MODIS. Figures 4.29 and 4.30 present the KDE plots and boxplots of the differences between the L2 LST. The first column displays the L2 differences using KDE plots, including the mean and standard deviation: blue curves represent the L2 differences

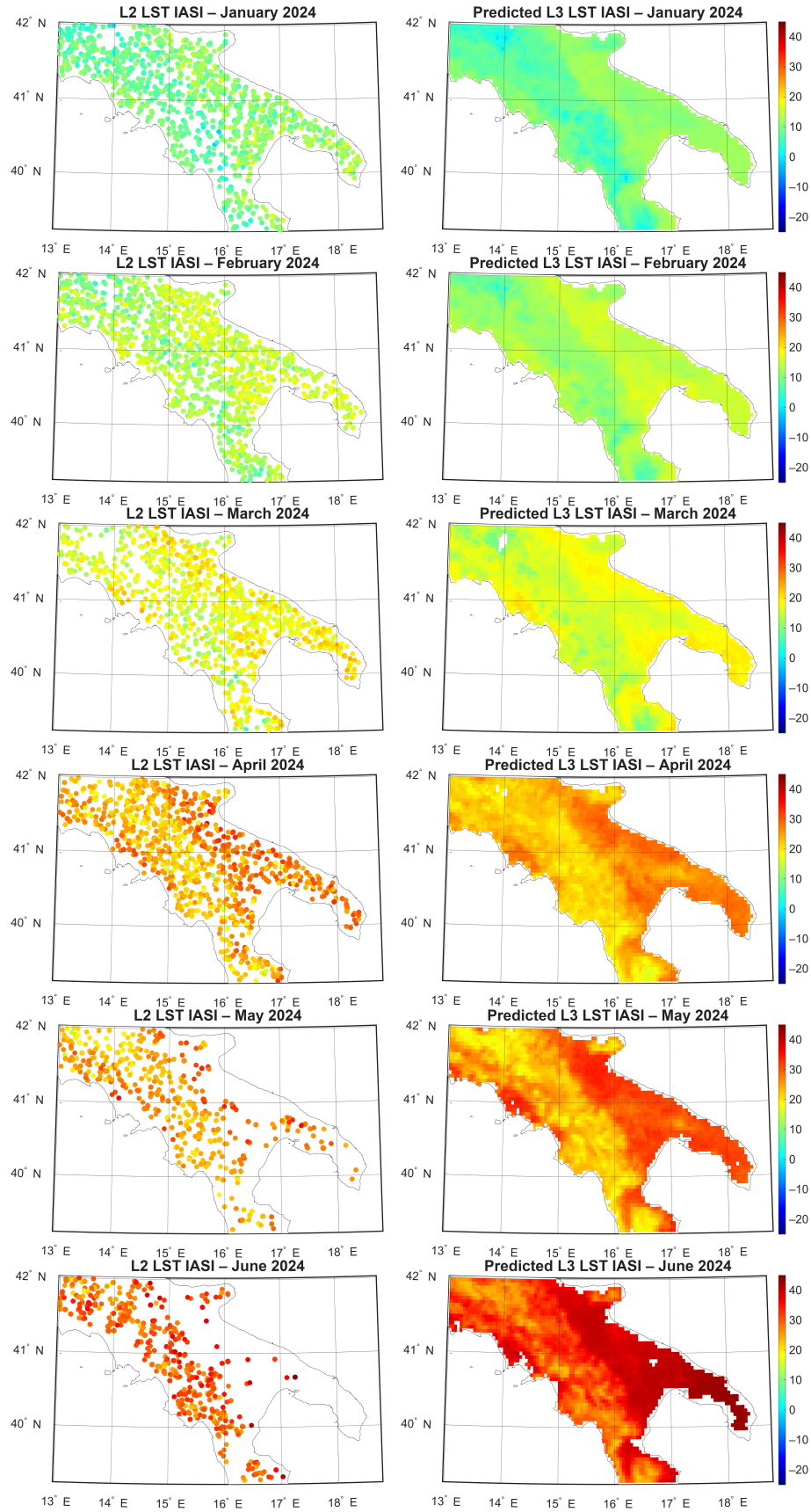


Figure 4.24: Daytime L3 LST maps over the Basilicata region for January–June 2024. Left: IASI L2 observations. Right: L3 LST predicted using Stacked Regression; each row represents a month.

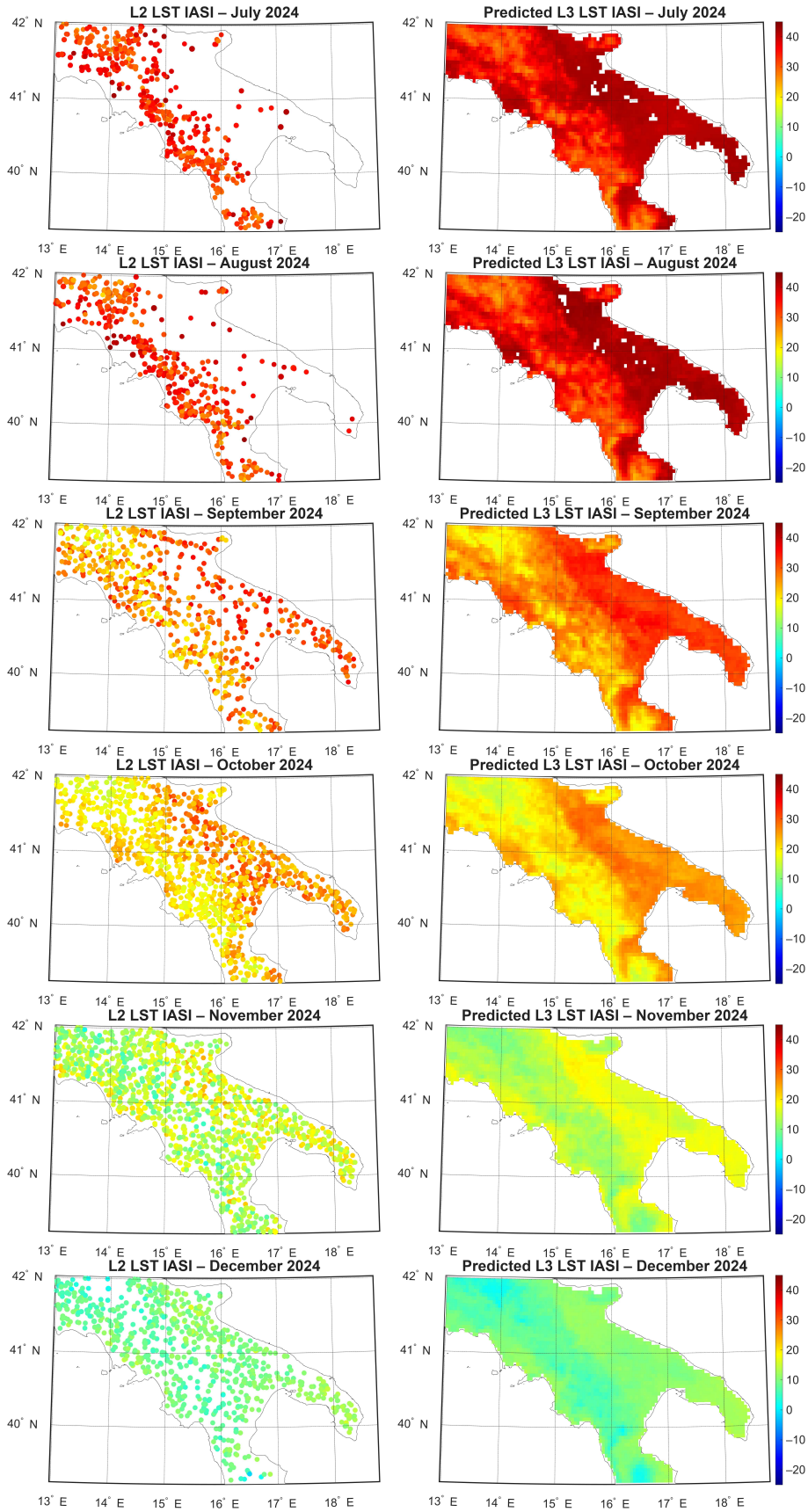


Figure 4.25: Daytime L3 LST maps over the Basilicata region for July–December 2024. Left: IASI L2 observations. Right: L3 LST predicted using Stacked Regression; each row represents a month.

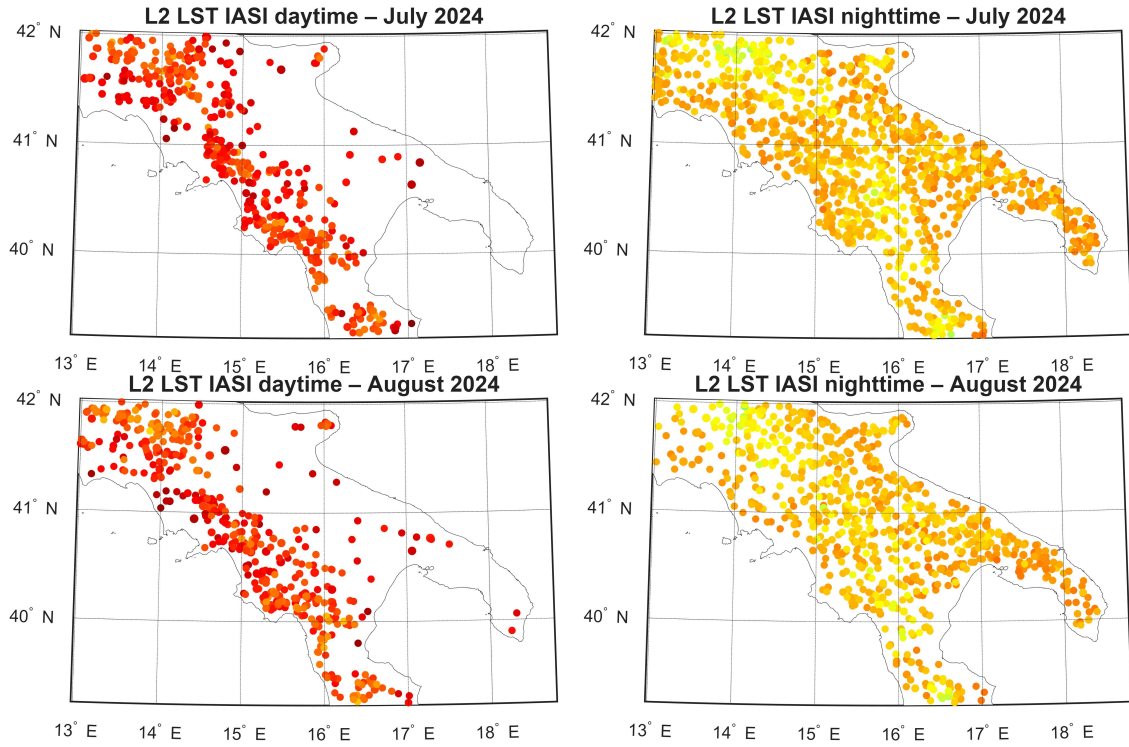


Figure 4.26: Daytime and nighttime L2 LST maps for July and August 2024.

between IASI and AVHRR, red curves represent those between IASI and SEVIRI, and yellow curves represent those between IASI and MODIS. The second column shows the same differences using boxplots, with the corresponding R^2 coefficients indicated on the x -axis.

The LST derived from AVHRR shows the highest agreement with IASI, exhibiting the largest R^2 values (with the only exceptions of January and December) and the lowest standard deviation ($<1.84^\circ\text{C}$). The bias results are mixed: in some months, AVHRR shows the lowest bias, while in others, the other sensors have lower values. However, the AVHRR bias is more consistent, remaining positive and close to 1°C . Similar to the Po Valley, SEVIRI shows a seasonal pattern, with a negative bias in winter and a strong positive one in summer, while this seasonality is less evident in MODIS. Between SEVIRI and MODIS, there is no clear winner in terms of R^2 , which varies depending on the month.

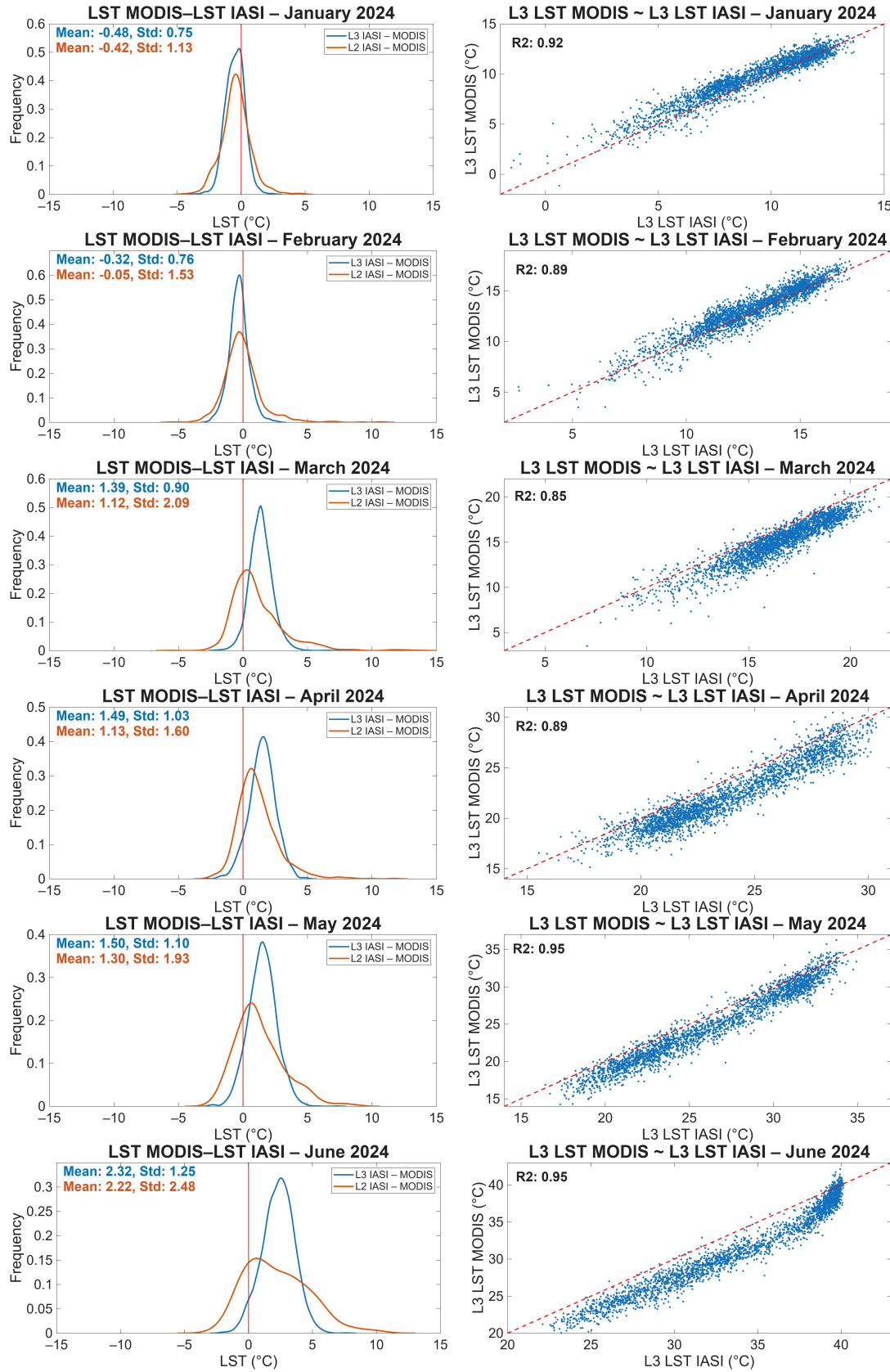


Figure 4.27: Daytime L2/L3 differences (IASI – MODIS) over the Basilicata region for January–June 2024. Left: KDE plots of the L2/L3 differences (red and blue), including mean and standard deviation. Right: scatterplots between predicted IASI and MODIS L3 LST values with the coefficient of determination (R^2).

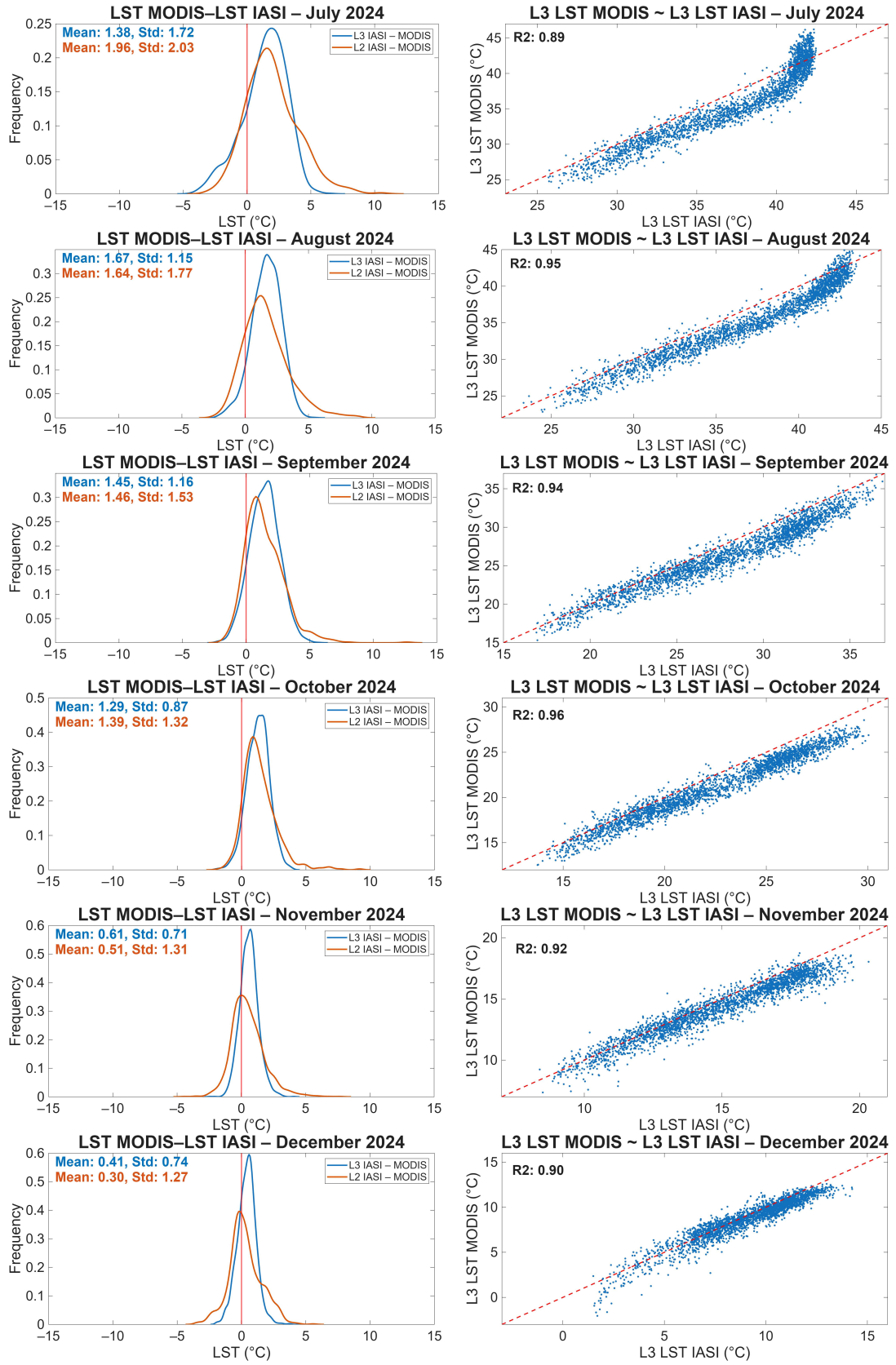


Figure 4.28: Daytime L2/L3 differences (IASI – MODIS) over the Basilicata region for July–December 2024. Left: KDE plots of the L2/L3 differences (red and blue), including mean and standard deviation. Right: scatterplots between predicted IASI and MODIS L3 LST values with the coefficient of determination (R^2).

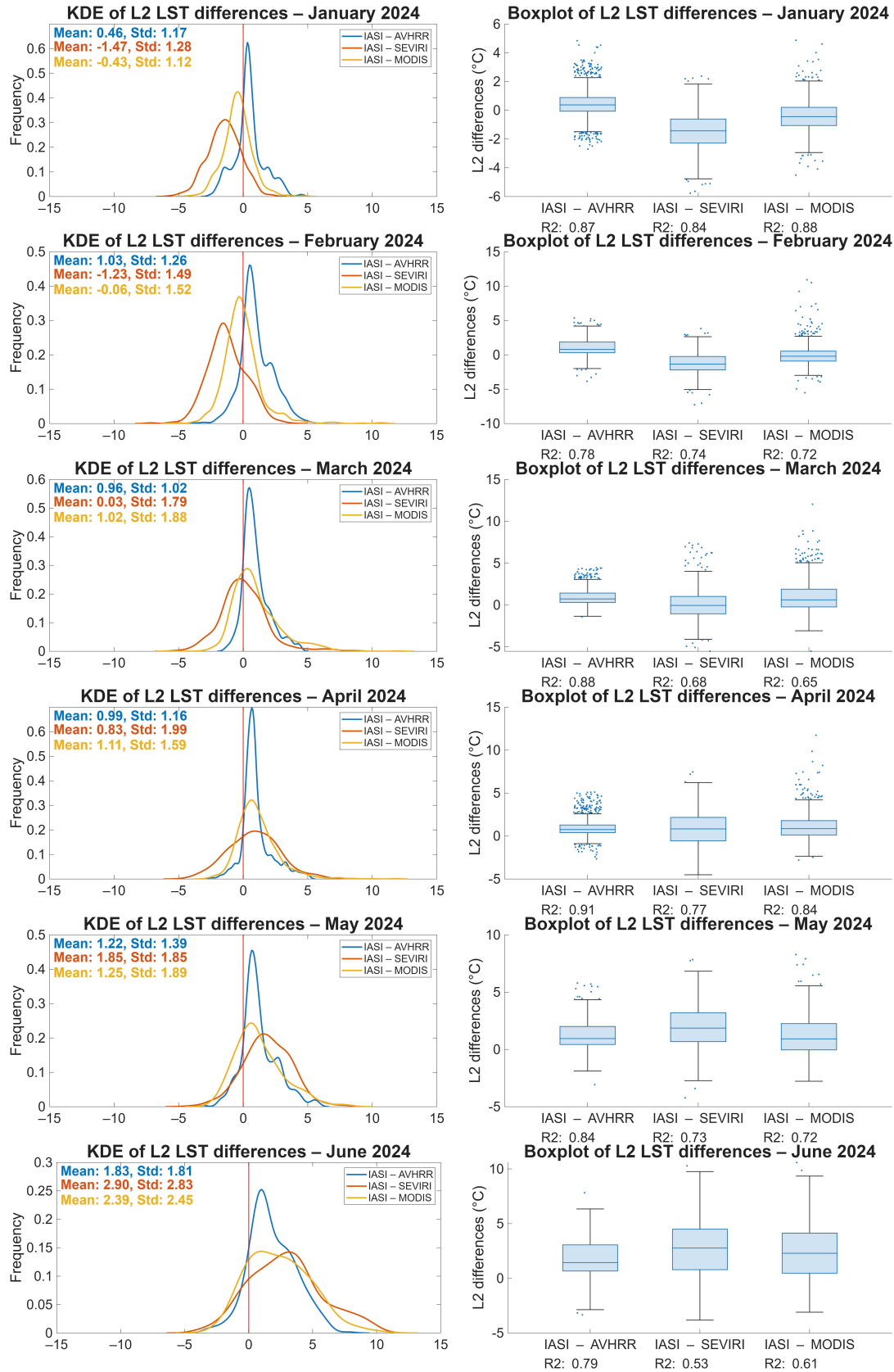


Figure 4.29: Daytime comparison of LST from IASI, AVHRR, SEVIRI, and MODIS for January–June 2024. Left: KDE plots of L2 differences (blue: AVHRR, red: SEVIRI, yellow: MODIS), including mean and standard deviation. Right: boxplots of the same differences with corresponding R^2 values on the x -axis.

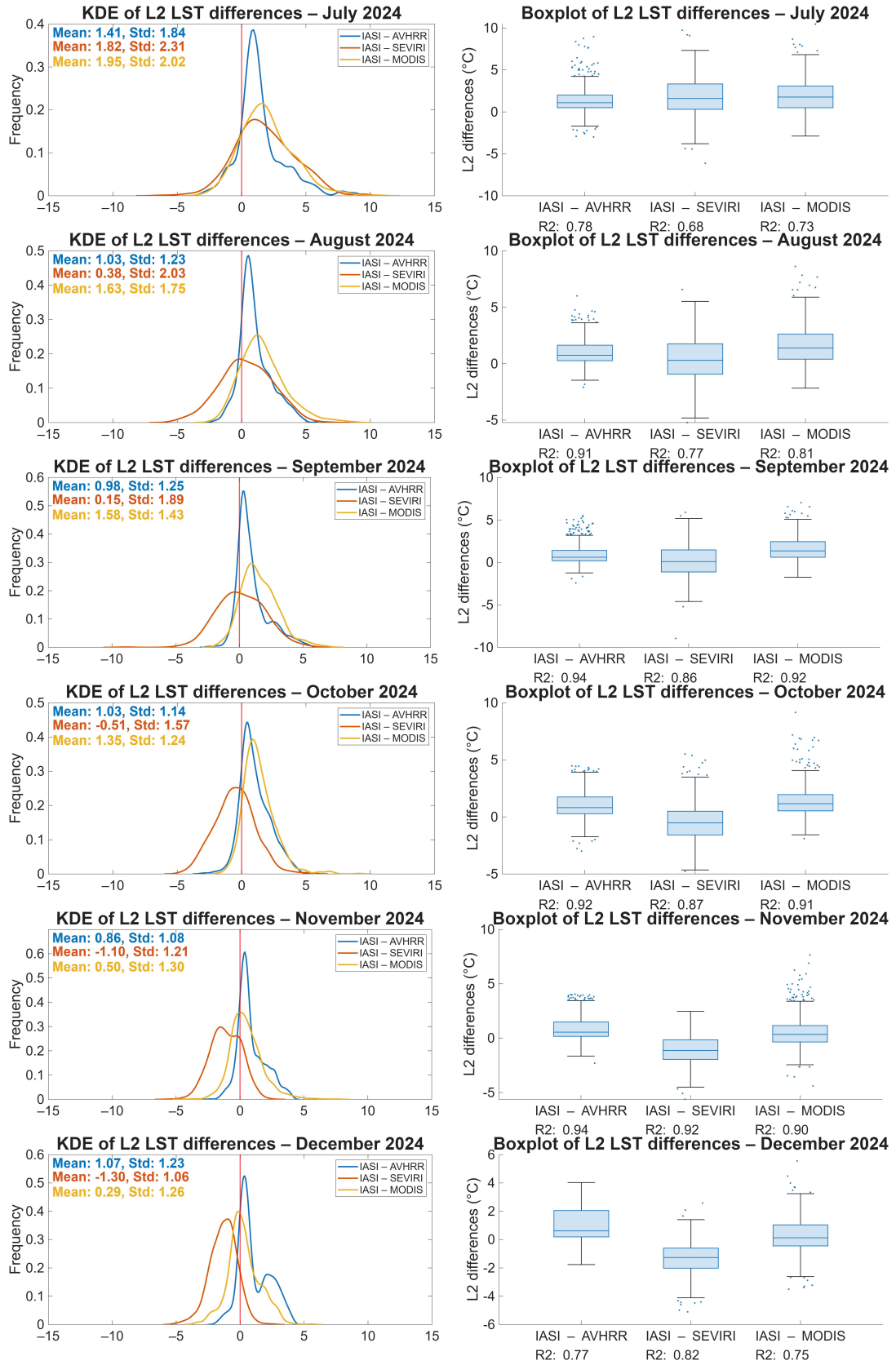


Figure 4.30: Daytime comparison of LST from IASI, AVHRR, SEVIRI, and MODIS for July–December 2024. Left: KDE plots of L2 differences (blue: AVHRR, red: SEVIRI, yellow: MODIS), including mean and standard deviation. Right: boxplots of the same differences with corresponding R^2 values on the x -axis.

4.5.2 T_d

Figures 4.31 and 4.32 present the monthly MAE and RMSE of T_d for the Basilicata region during daytime and nighttime overpasses, respectively. GBT, again, achieved the best performance

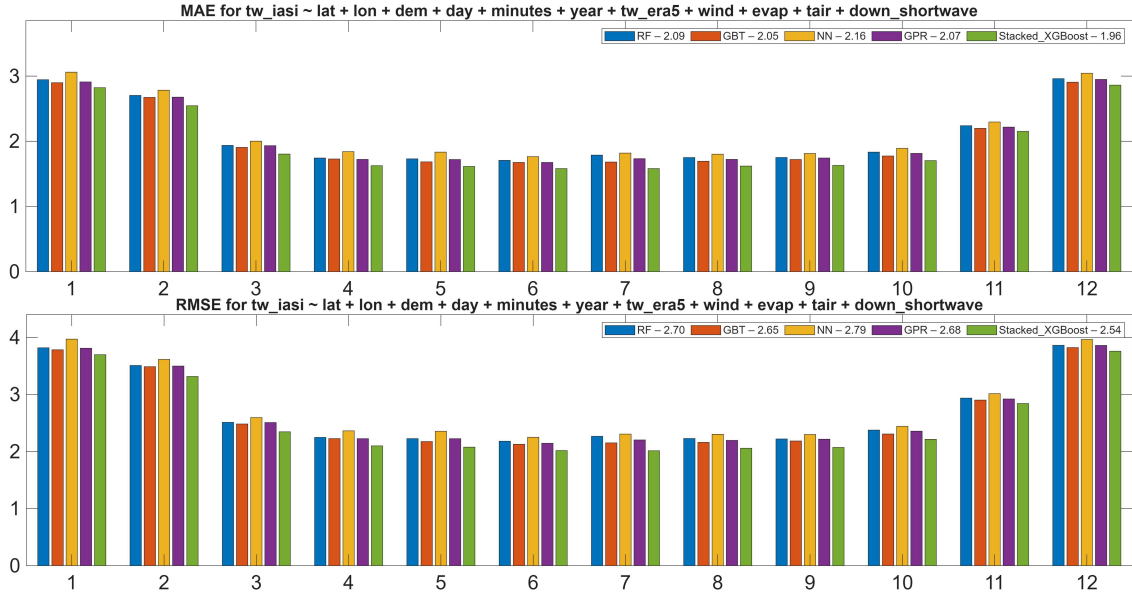


Figure 4.31: Cross-validated MAE (top) and RMSE (bottom) of T_d for the tested ML algorithms during daytime overpasses: RF (blue), GBT (orange), NN (yellow), GPR (purple), and Stacked Regression (green). Numbers in the legend represent the average MAE and RMSE across all months.

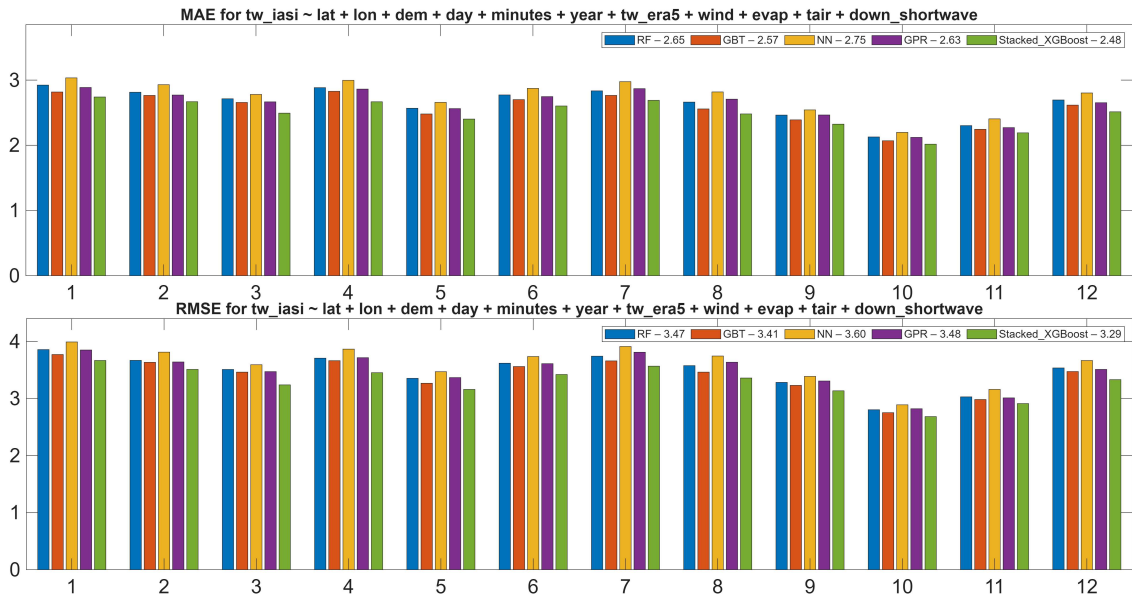


Figure 4.32: Cross-validated MAE (top) and RMSE (bottom) of T_d for the tested ML algorithms during nighttime overpasses: RF (blue), GBT (orange), NN (yellow), GPR (purple), and Stacked Regression (green). Numbers in the legend represent the average MAE and RMSE across all months.

among the tested ML algorithms, with an MAE of 2.05 °C and an RMSE of 2.65 °C for daytime overpasses, and an MAE of 2.57 °C and an RMSE of 3.41 °C for nighttime overpasses. Stacked Regression further improved the performance: MAE and RMSE decreased to 1.96 °C and 2.54 °C for daytime data, and to 2.48 °C and 3.29 °C for nighttime data, corresponding to improvements of 4.3% and 3.5%, respectively. Nighttime conditions are confirmed to be more challenging.

Figures 4.33 and 4.34 show the L3 T_d maps for 2024 at 0.05° spatial resolution.

As expected, the T_d maps for the Basilicata region also appear smoother than the LST ones, showing smaller variations both across months and spatially. However, the validation of T_d with ARPA data confirms the high consistency of the interpolated product. For the Basilicata region, six ARPA stations were used in the validation step, and Figure 4.35 shows daytime time-series plots of T_d from ARPA (blue), IASI (red), and ERA5 (green) for four of them, together with their corresponding Pearson correlation coefficients. Correlations are also very high, with the L3 IASI product even slightly outperforming ERA5.

Figure 4.36 shows the overall validation of T_d using all six ARPA stations. The validation is performed for both daytime (first row) and nighttime overpasses (second row). ARPA T_d is compared with IASI L3 T_d (first column), ERA5 T_d (second column), and IASI L2 T_d (third column). For each comparison, the Pearson correlation coefficient, bias, and RMSE were computed.

The downscaled IASI T_d shows a very high agreement with ARPA stations, with correlation coefficients of 0.94 for daytime and 0.92 for nighttime, higher than those obtained for the Po Valley. When compared to ERA5, the L3 IASI product shows comparable performance—better during the daytime and slightly worse at night. Moreover, the L3 IASI exhibits a lower bias than ERA5, with absolute values below 1 °C during the day and around 2 °C at night. The only difference lies in the bias sign, which is always positive here, whereas it was negative over the Po Valley. As before, the RMSE remains higher for IASI. When also considering the IASI L2 data, the interpolated product shows lower bias, higher correlation, and reduced RMSE, confirming the improvement achieved through the proposed downscaling approach.

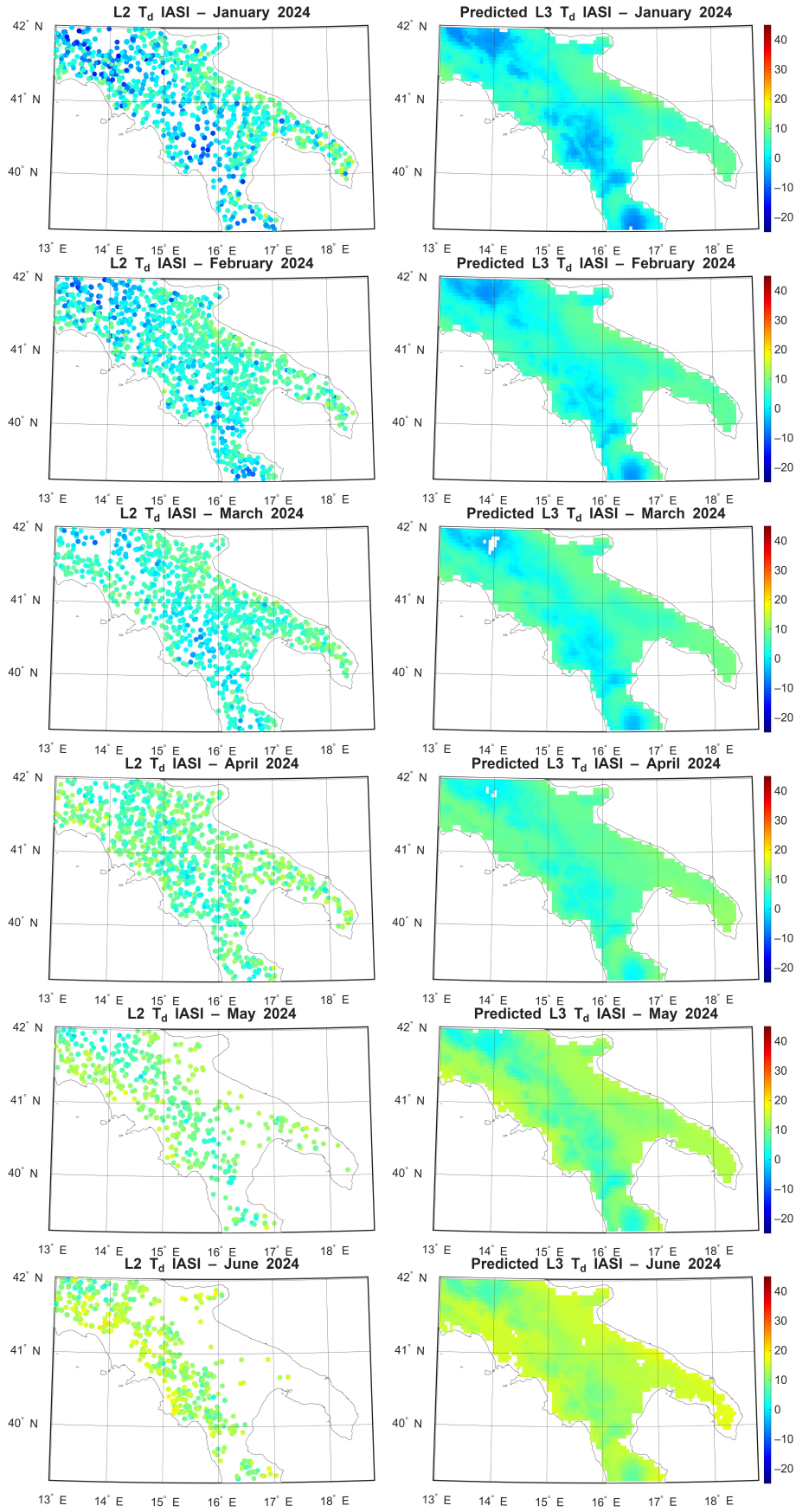


Figure 4.33: Daytime L3 T_d maps over the Basilicata region for January–June 2024. Left: IASI L2 observations. Right: L3 T_d predicted using Stacked Regression; each row represents a month.

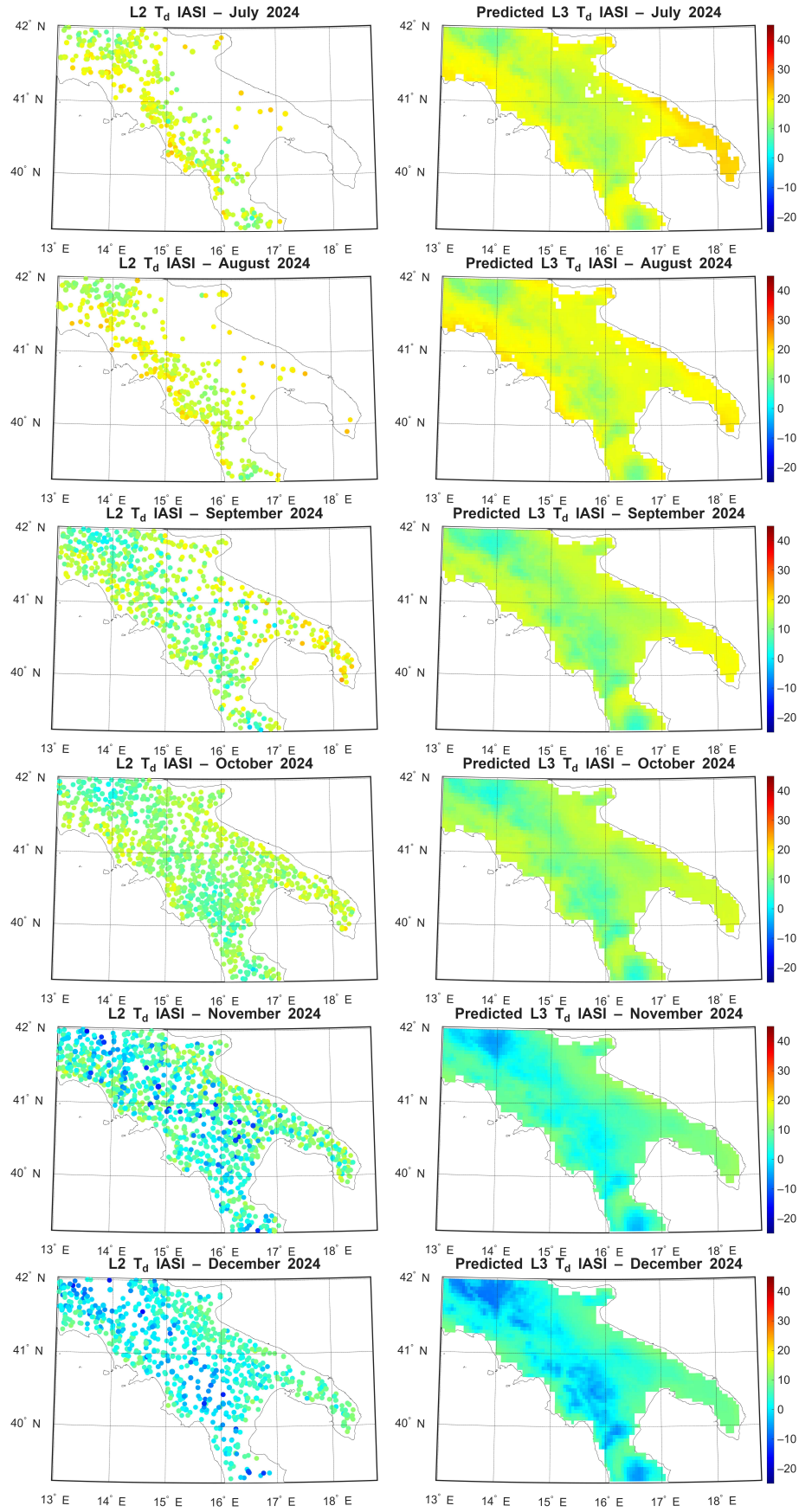


Figure 4.34: Daytime L3 T_d maps over the Basilicata region for July–December 2024. Left: IASI L2 observations. Right: L3 T_d predicted using Stacked Regression; each row represents a month.

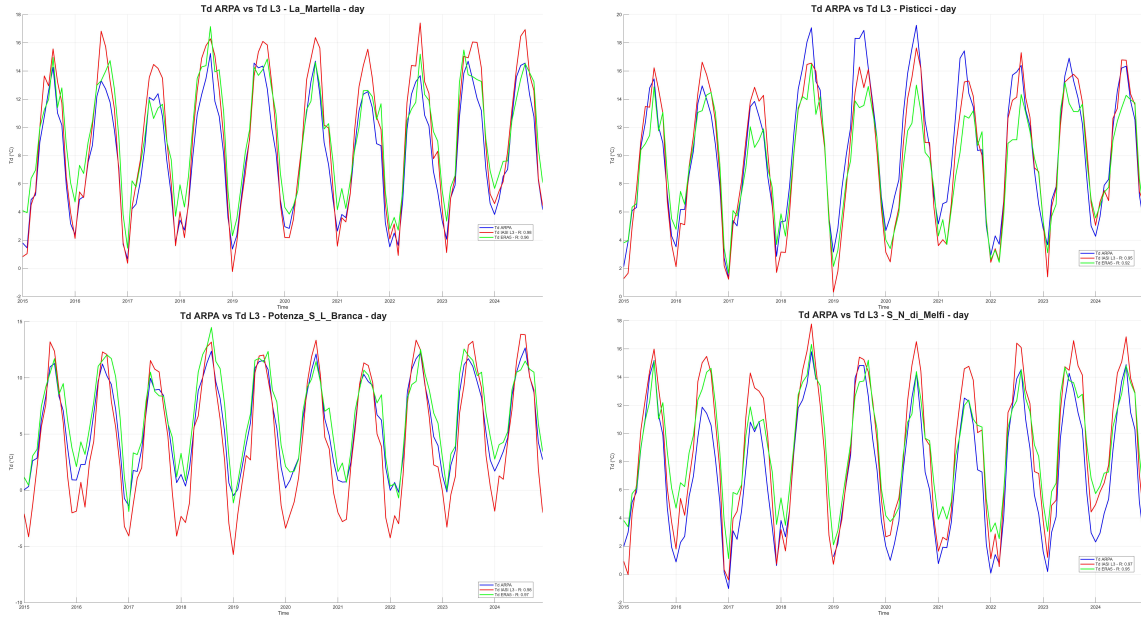


Figure 4.35: Daytime T_d time-series from ARPA (blue), IASI (red), and ERA5 (green) for four representative stations in the Basilicata region.

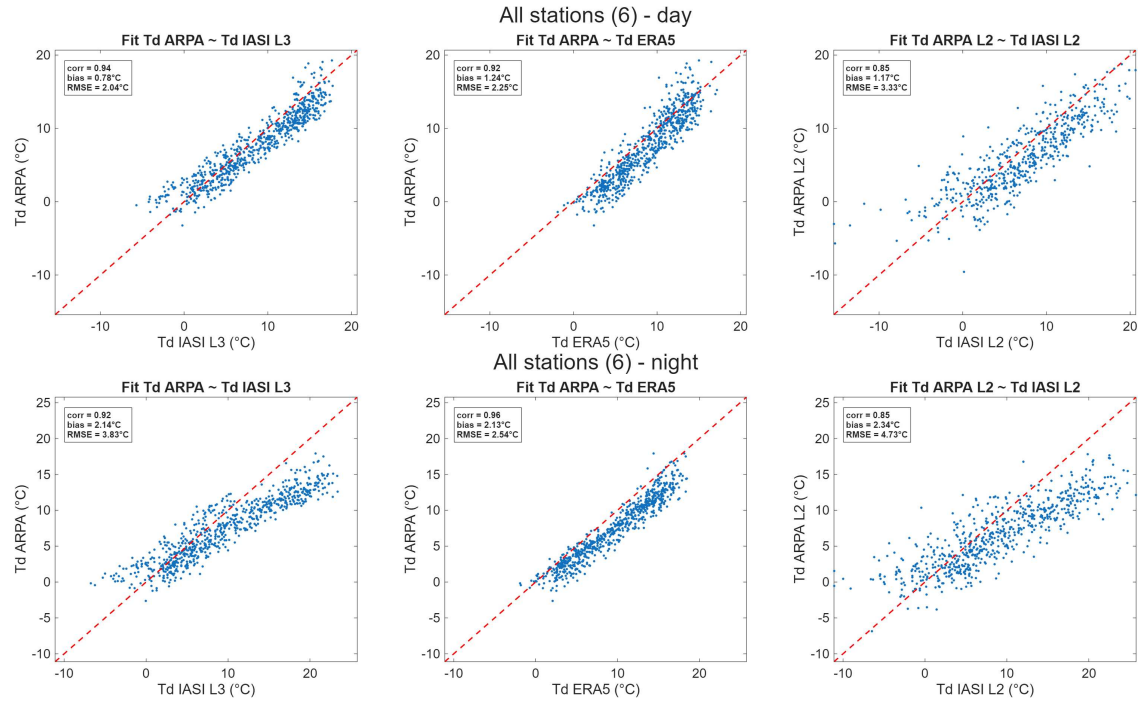


Figure 4.36: Validation of T_d using all 6 ARPA stations over the Basilicata region. The first and second rows correspond to daytime and nighttime overpasses, respectively. Columns show the comparison of ARPA T_d with IASI L3 (left), ERA5 (centre), and IASI L2 (right). Pearson correlation, bias, and RMSE are reported for each case.

4.5.3 WDI

Figure 4.37 shows the daytime L3 WDI maps for 2024 at a spatial resolution of 0.05° . Here again, the WDI highlights areas that are not easily distinguishable from the LST and T_d alone. For example, in summer, the WDI highlights the influence of the sea along the Tyrrhenian coast. Although LST is high, the index shows lower values, reflecting the additional moisture supplied by the sea.

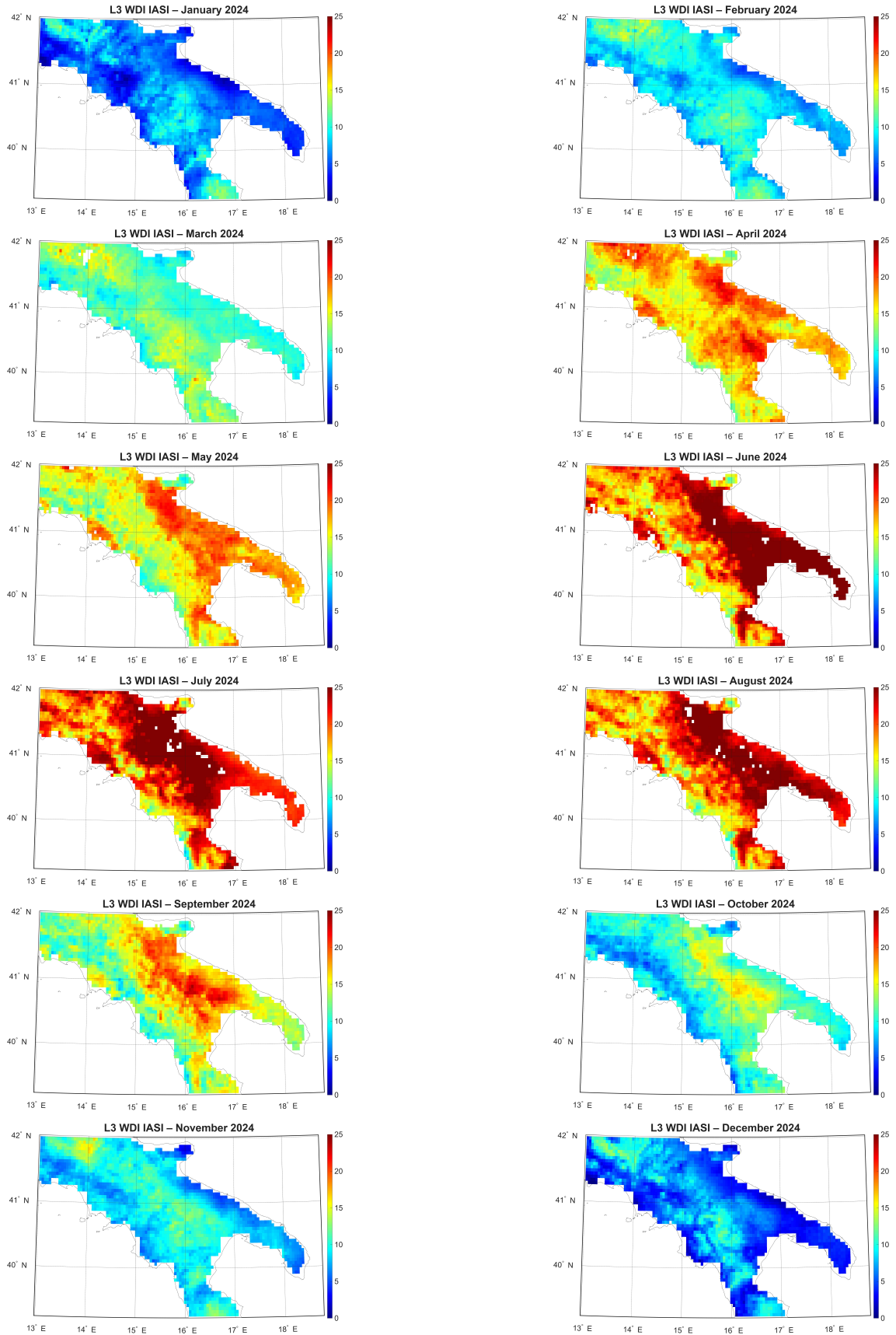


Figure 4.37: Daytime L3 WDI maps over the Basilicata region for 2024 computed as the difference between the IASI L3 LST and T_d .

To identify the years with the highest water deficit, Figure 4.38 shows the seasonal distribution of WDI values for each year, restricting the analysis to the areas depicted in Figure 4.3. The years with the highest WDI values (in decreasing order) are 2017, 2024 and 2022. This is again confirmed by the temperature and precipitation anomalies, since southern Italy recorded the highest temperatures and lowest precipitation levels during these years. Another example is the year 2018, which registered the lowest WDI within the reference period: although it was still the fourth warmest year, it also experienced the highest precipitation levels. As in the Po Valley, the WDI successfully captured the years associated with water stress events also in the Basilicata region.

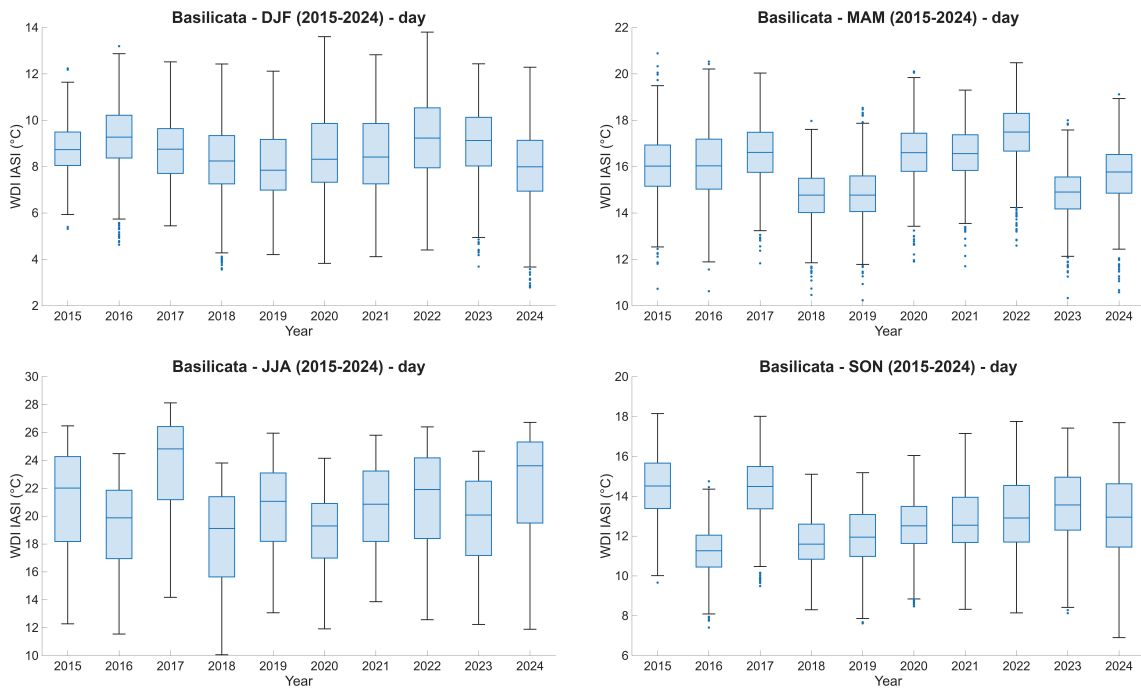


Figure 4.38: Daytime seasonal WDI boxplots over the Basilicata region by year. Each boxplot represents the distribution of WDI values selected according to the defined criteria within the Basilicata region.

Similarly to the Po Valley, the WDI was also compared with SSM and NDMI for the Basilicata region. The comparison was restricted to two representative cases: May and June 2024 (Figure 4.39) and June 2022 and 2023 (Figure 4.40).

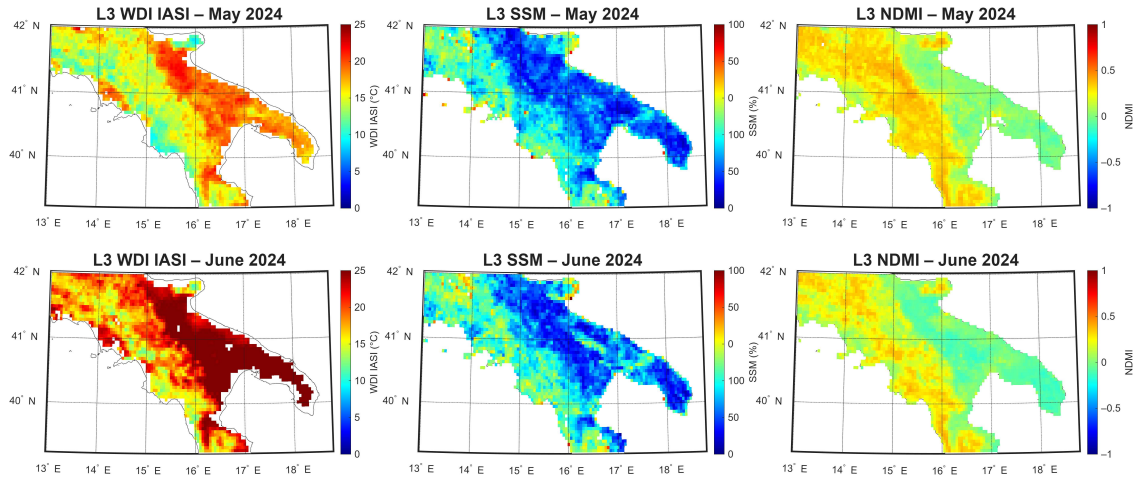


Figure 4.39: Comparison between daytime WDI, SSM and NDMI for May (top) and June (bottom) 2024 over the Basilicata region.

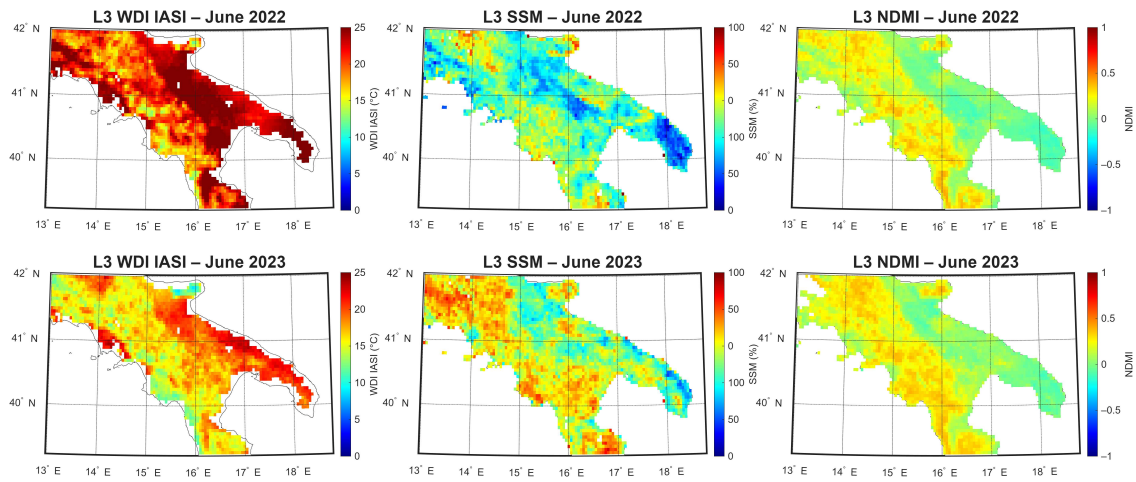


Figure 4.40: Comparison between daytime WDI, SSM and NDMI for June 2022 (top) and June 2023 (bottom) over the Basilicata region.

Figure 4.39 shows the comparison for May and June 2024 where May recorded above-average precipitation levels, while June experienced an intense precipitation deficit[59]. The WDI captured this pattern well, showing much higher values in June. Conversely, the difference in SSM between the two months is negligible, indicating that it failed to capture this change. Interestingly, the NDMI better agrees with WDI as the differences between the two months are evident and areas with low WDI correspond to high NDMI values, and vice versa. This suggests that even if soil moisture conditions were similar between the two months, vegetation faced water stress only in June, a feature effectively captured by the WDI.

Next, Figure 4.40 presents the comparison for June 2022 and 2023, when 2022 was much hotter and drier than 2023 [57, 58]. This is again confirmed by the WDI, which shows values up to 10 °C higher in 2022. The same trend is observed in both NDMI and SSM, with 2022 showing a greater plant water deficit and lower soil moisture content.

Chapter 5

WDI projections

Understanding how vegetation water stress may evolve under climate change requires more than a snapshot of recent events. It is important to identify long-term trends and determine whether it is becoming a more frequent event. Future climate projections provide a key tool for this analysis. Projecting WDI allows translating modelled changes in temperature and humidity into a metric more closely tied to vegetation stress and compound heat–dryness episodes.

In this chapter results on WDI projections on the two target areas are presented. Specifically, Section 5.1 describes what climate projections are, Section 5.2 and Section 5.3 contain the description of the Coupled Model Intercomparison Project (CMIP) and the Coordinated Regional Climate Downscaling Experiment (CORDEX), while Sections 5.2 and Section 5.5 provide the results.

5.1 Climate projections

Assessing climate risks requires not only short-term forecasts but also long-term projections of how the climate might change under different scenarios. It is important to distinguish between climate predictions and climate projections.

Climate predictions refer to the short-term forecasting of climate conditions based on the current state of the climate system and its known patterns of variability. These predictions usually span a few months to a few years and aim to **forecast** specific climate phenomena, such as seasonal weather patterns, temperature anomalies, and precipitation trends. They are based on a combination of observations, statistical models, and physical knowledge of climate dynamics with the goal of providing accurate information for particular regions and seasons.

Climate projections, on the other hand, analyse long-term simulations of potential future climate conditions under different greenhouse gas emission scenarios and socio-economic pathways. These projections extend over decades to centuries and present possible scenarios of how the climate could change under different assumptions about human activity and natural processes. Climate projections do not try to predict individual weather events, but rather provide a plausible "what if" scenario illustrating a possible future climate, supporting policymakers and researchers in designing effective climate adaptation and mitigation strategies.

Climate projections are based on different **Global Climate Models (GCMs)**. A GCM is a

mathematical model that simulates the physics of the major climate systems, including atmosphere, ocean, land surface, and cryosphere [192]. The first working GCM was created in 1956 by Norman A. Phillips [188]. The model, which had a spatial resolution of 375 km, was run on an IAS computer with just 1 kB of main memory and 2 kB of storage. Since then, researchers from several institutions around the world have continually developed GCMs to build efficient and reliable models for simulating climate systems [52], allowing scientists to make more detailed projections.

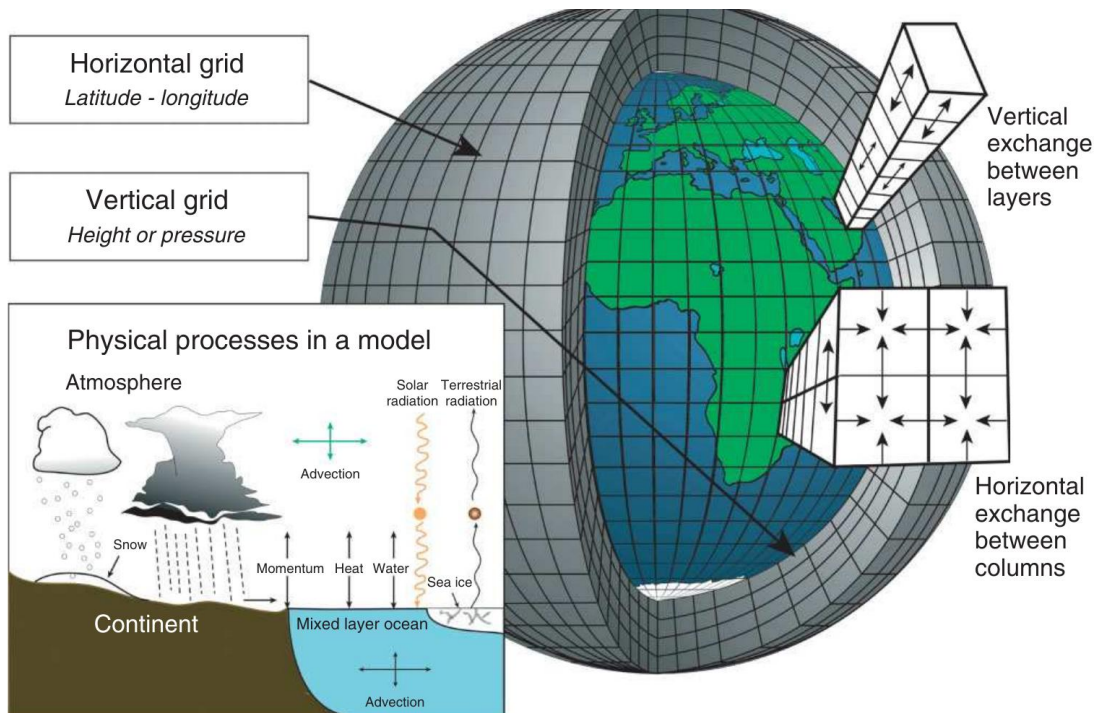


Figure 5.1: Schematic representation of the Cartesian grid structure used in GCMs. Each of the thousands of 3-dimensional grid cells can be represented by mathematical equations that describe the materials in it and the way energy moves through it. Source: Edwards, P. (2011) [52]

However, each GCM produces different simulations because they rely on different inputs, numerical approximations, physical equations, parameterisations and spatial and temporal resolutions. Different outputs do not necessarily mean that one GCM is universally better than another, but rather that it could perform better in some regions of the world and worse in others. The perfect GCM does not exist. The well-known aphorism by George E. P. Box “all models are wrong, but some are useful” is particularly true for climate models. For this reason, scientists usually use a combination of different GCMs and/or multiple runs of a single GCM with different setups. This approach is called **ensemble** and should produce a more reliable and meaningful outcome.

Climate projections rely on one or more GCMs that simulate the climate over many years, usually up to the end of the century. In these simulations, GCMs are run with input parameters that reflect a wide range of possible changes in future anthropogenic greenhouse gas emissions/concentrations. Multiple scenarios are considered, each corresponding to a different level

of **radiative forcing**. According to the Intergovernmental Panel on Climate Change (IPCC), the radiative forcing is "the change in the net, downward minus upward, radiative flux (expressed in W/m^2) due to a change in an external driver of climate change, such as a change in the concentration of carbon dioxide (CO_2), the concentration of volcanic aerosols or the output of the Sun"[107].

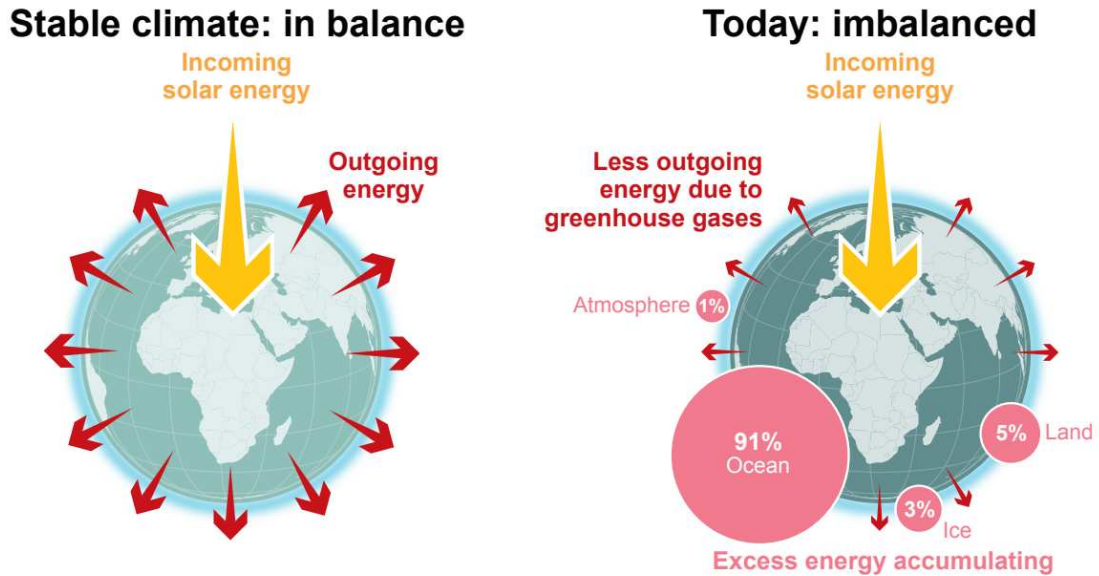


Figure 5.2: The Earth's energy budget describes the balance between incoming and outgoing energy in the climate system. Since at least the 1970s, less energy is flowing out than is flowing in, which leads to excess energy being absorbed by the ocean, land, ice and atmosphere, with the ocean absorbing 91%. Source: IPCC [108]

A planet is in radiative equilibrium when the absorbed energy (mostly from its star, e.g. the Sun) equals the energy it emits back to space (mostly as infrared radiation). In this state, the planet's energy budget is balanced: it is in radiative equilibrium with a net zero radiative forcing. However, if radiative forcing is not zero, for example if it is positive, more energy is coming in than going out from the planet. In response to these forcings, the planet system will warm until it has restored the balance through changes in the amount of outgoing thermal radiation (the warmer the planet, the more radiation it emits). We say that it has reached a **higher equilibrium temperature**. To compute the radiative forcing, values from 1750, i.e. prior to the industrial era, are generally used as a baseline. In 2024 the human-caused radiative forcing was estimated to be around $2.97 \text{ W}/\text{m}^2$, mainly due to increased Greenhouse Gas (GHG) concentrations, partly reduced by cooling due to increased aerosol concentrations [68]. Figure 5.3 from the latest IPCC Sixth Assessment Report (AR6) [109] clearly highlights the different components (both positive and negative) considered in the calculation of the radiative forcing. The components responsible for the observed global warming, depicted in panel (a), are detailed in panel (b) and (c). Specifically, panel (b) shows that nearly the entire contribution to temperature changes arises from human

activities, while natural contributions (solar and volcanic drivers) are almost zero. Panel (c) presents the temperature changes from individual human-related components, with the highest contribution given by CO₂ and CH₄.

Observed warming is driven by emissions from human activities, with greenhouse gas warming partly masked by aerosol cooling

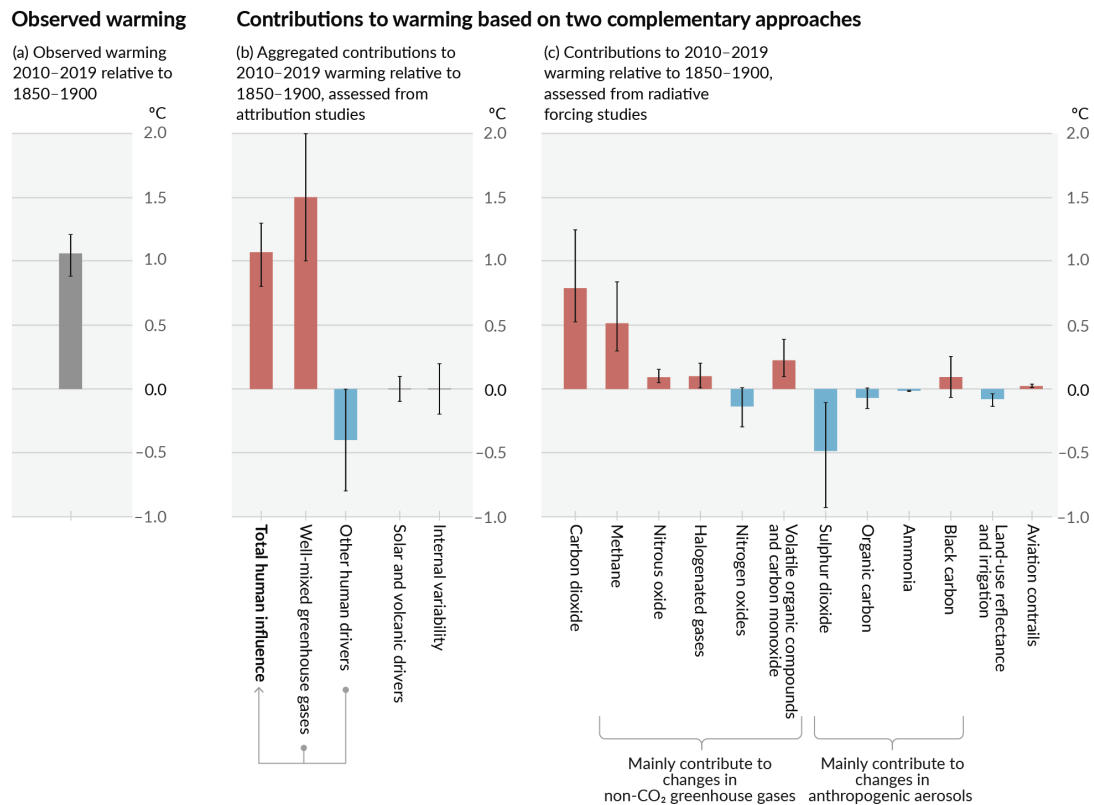


Figure 5.3: Panel (a) shows the observed global warming (increase in global surface temperature). Panel (b) presents evidence from attribution studies, which synthesise information from climate models and observations. The panel shows temperature changes attributed to: total human influence; changes in well-mixed greenhouse gas concentrations; other human drivers due to aerosols, ozone and land-use change (land-use reflectance); solar and volcanic drivers; and internal climate variability. Panel (c) provides evidence from the assessment of radiative forcing and climate sensitivity. The panel shows temperature changes from individual components of human influence: emissions of greenhouse gases, aerosols and their precursors; land-use changes (land-use reflectance and irrigation); and aviation contrails. Source: IPCC [108]

5.2 The Coupled Model Intercomparison Project (CMIP)

A major step forward in climate projections came with the foundation of the **Coupled Model Intercomparison Project (CMIP)** in 1995. CMIP is a project of the World Climate Research

Programme (WCRP) that provides climate projections to understand past, present and future climate change. It was designed to give climate scientists access to a database of coupled global model simulations following standard experiment protocols. These simulations were used to understand why different models produce different results, even under identical model input, and to identify results consistently reproduced across models [242]. CMIP is organised in phases, each phase with new and improved climate model experiment protocols, standards, and data distribution mechanisms. From the first two phases, CMIP1 and CMIP2, which included only 18 GCMs, the most recent phase, CMIP6, comprises more than 100 GCMs from nearly 50 institutions [53]. The next phase, CMIP7, is currently under development and is expected to be released soon.

One of CMIP's major contributions is the use of standardised GHG concentration pathways. In each phase, different global emissions projection datasets have been used to drive GCMs projections. For example, CMIP5 [223], initiated in 2008, uses the Representative Concentration Pathways (RCPs). The RCPs are climate change scenarios formally adopted by the IPCC that describe future greenhouse gas concentrations. RCPs follow the naming convention RCP x, where x refers to the radiative forcing level in 2100. For example, RCP 4.5 corresponds to a radiative forcing of 4.5 W/m^2 . Under CMIP5, four scenarios are available: RCP 2.6, RCP 4.5, RCP 6.0, and RCP 8.5.

With **CMIP6**, started in 2016, radiative forcing scenarios were improved also including the socioeconomic scenarios with the **Shared Socioeconomic Pathways (SSPs)**. SSPs follow the naming convention SSPx-y, where x refers to the socioeconomic storyline and y refers to the radiative forcing level in 2100. For example, SSP2-4.5 uses the second socioeconomic scenario (SSP2), called *Middle of the road*, with a radiative forcing of 4.5 W/m^2 . Following the SSP narratives provided by O'Neill [195], the SSP2 is described as:

“The world follows a path in which social, economic, and technological trends do not shift markedly from historical patterns. Development and income growth proceeds unevenly, with some countries making relatively good progress while others fall short of expectations. Global and national institutions work towards but make slow progress in achieving sustainable development goals. Environmental systems experience degradation, although there are some improvements and overall the intensity of resource and energy use declines. Global population growth is moderate and levels off in the second half of the century. Income inequality persists or improves only slowly and challenges to reducing vulnerability to societal and environmental changes remain.”

The interested reader can find the full set of SSP narratives in O'Neill *et al.* [195].

Both RCP and SSP are defined by their radiative forcing level in 2100. However, the SSP also includes the socioeconomic context, examining various scenarios that consider technological, social and political developments as well as climate-related challenges. From the four baseline scenarios introduced with CMIP5, CMIP6 introduced four new “gap” scenario that define forcing pathways not represented by the RCPs, thereby addressing new questions of interest for integrated

analysis [179]. Among these eight scenarios, only SSP1-2.6, SSP2-4.5, SSP3-7.0, and SSP5-8.5 are considered the main ones. These so-called “Tier 1” scenarios are required for any climate model to participate in CMIP6, while the remaining four scenarios (SSP1-1.9, SSP4-3.4, SSP5-3.4-OS and SSP4-6.0) are “Tier 2” and are optional. Linking SSPs and RCPs provides a comprehensive picture of the interactions between socioeconomic trends and climate factors. Figure 5.4, adapted from O’Neill (2016) [179], summarises all CMIP6 scenarios and compares them with the earlier CMIP5 RCPs.

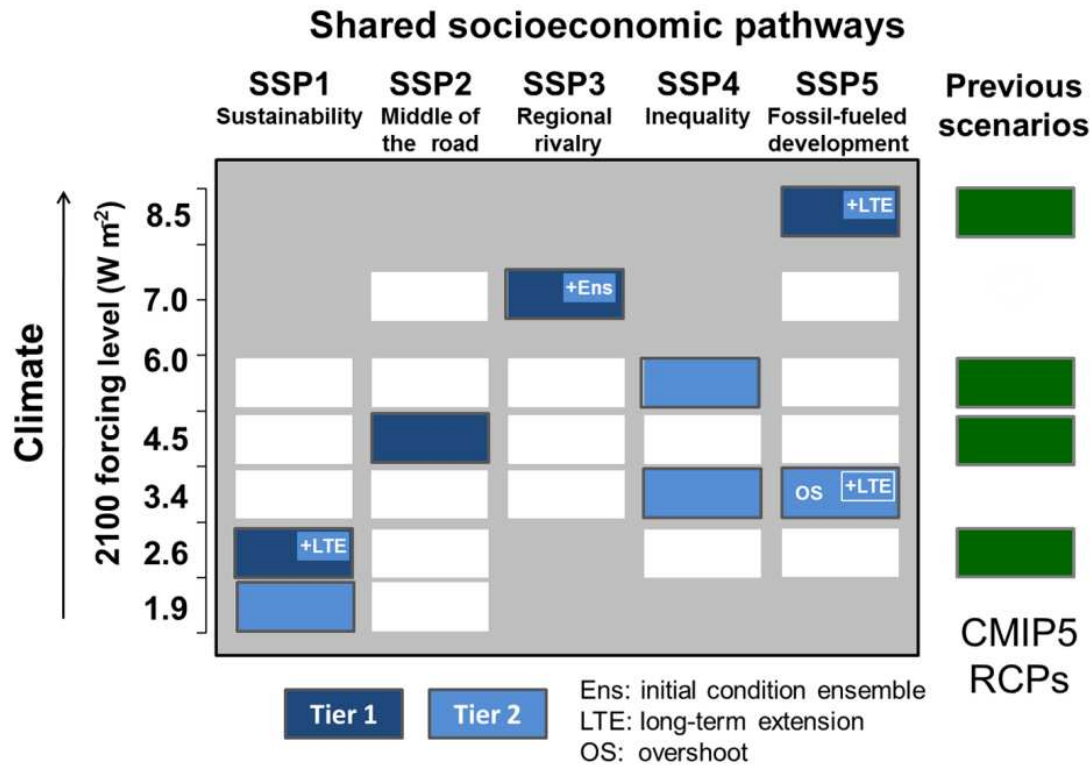


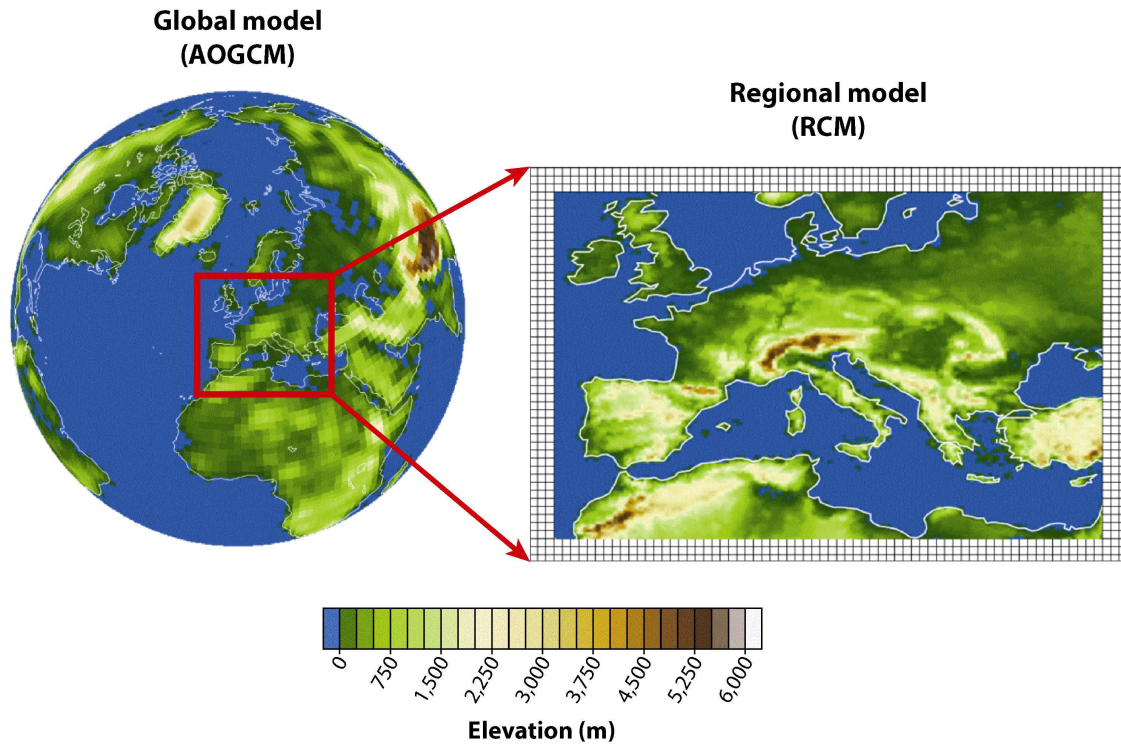
Figure 5.4: SSP-RCP scenario matrix illustrates ScenarioMIP simulations where each cell indicates a combination of a SSP and a radiative forcing. Dark blue cells indicate “Tier 1” scenarios; light blue cells indicate “Tier 2” scenarios; white cells indicate scenarios for which climate information is intended to come from the SSP scenario to be simulated for that row; green cells show the old CMIP5 RCP scenarios for comparison. Source: IPCC [108]

5.3 Dynamical Downscaling and the CORDEX initiative

The problem with most GCMs is that they operate at coarse spatial resolutions, which at best reach 50 km. While this is sufficient for assessing global changes, it becomes inadequate for capturing local/regional climate variations. To overcome this limitation, GCMs are often downscaled to improve the spatial resolution.

Traditional downscaling methods are generally divided into two categories. **Statistical downscaling**, pioneered by Kim *et al.* (1984) [124], uses statistical or ML techniques to find relationships

between coarse and fine scale data, which are then applied to improve GCM outputs. **Dynamical downscaling**, pioneered by Giorgi and Bates (1989)[76], uses finer-scale physical models, such as **Regional Climate Models (RCMs)**, that take GCM outputs as boundary conditions to generate higher-resolution simulations over smaller spatial domains. Although computationally intensive, dynamical downscaling provides more detailed information about regional climate patterns while maintaining more physically consistent results. The advantages and limitations of dynamical downscaling are discussed in detail in Hong and Kanamitsu (2014) [93].



 Giorgi F, Gutowski Jr WJ. 2015.
Annu. Rev. Environ. Resour. 40:467–90

Figure 5.5: Schematic representation of the one-way RCM nesting technique, showing how RCMs improve the resolution of topography and coastlines. Source: Giorgi and Gutowski (2015) [77]

Many institutions have released dynamically downscaled products; however, these are frequently restricted by the number of years, climate scenarios, regions, and variables they cover. The main international reference framework for downscaling activities is the **Coordinated Regional Climate Downscaling Experiment (CORDEX)**, which was designed to better understand regional climate phenomena, improve and evaluate downscaling methods, and generate coordinated regional projections. Indeed, the goal of the CORDEX project is to provide an ensemble of high-resolution (0.22° , approximately 25 km) regional climate information. It covers almost the entire globe, divided into nine domains according to geographical region. In particular, two CORDEX domains, Med-CORDEX [201] and EURO-CORDEX [113], focus on the Mediterranean

basin and Europe, respectively. Europe is the only region with a sufficient number of simulations at a spatial resolution of 0.11° (approximately 12 km). North America has only a few simulations at this finer resolution, but the number is much smaller (118 products compared with 35,037 for Europe).

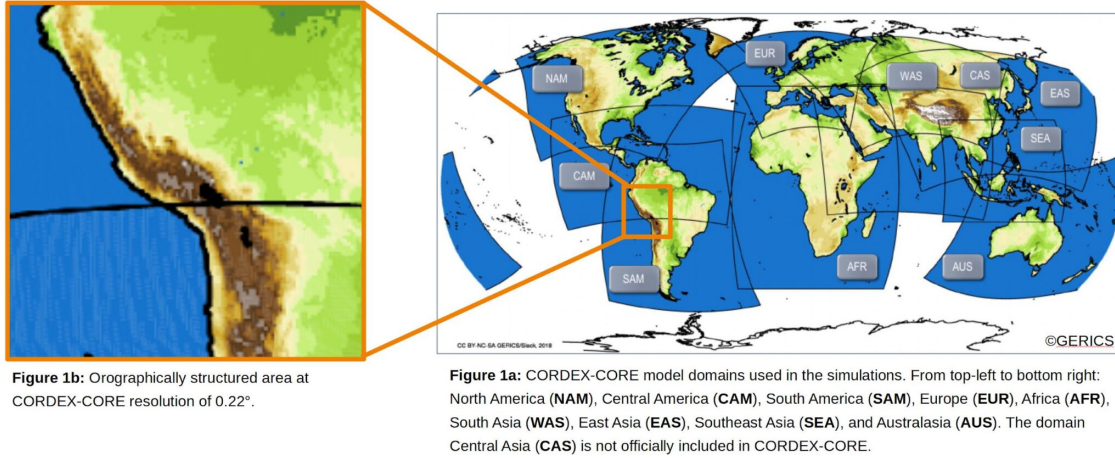


Figure 5.6: The nine model domains selected for the CORDEX-CORE ensemble. Source: CORDEX [189]

Unfortunately, the CORDEX initiative is not yet complete for CMIP6 (expected by the end of 2025), thus forcing the continued use of projections based on CMIP5. Still, another major limitation remains the relatively small number of simulations available, which may not sufficiently capture the full range of uncertainties associated with future climate projections. For example, the MED-CORDEX project has only two GCM–RCM combinations at 0.11° . On the other hand, the EURO-CORDEX domain offers more than 50 combinations, based on 6 GCMs and 14 RCMs, making it an ideal candidate for detailed regional climate studies.

5.4 WDI Projections: Methods and Workflow

Several studies have already analysed future climate projections in Europe, particularly in the Mediterranean basin, one of the most vulnerable regions to climate change with projections indicating reduced precipitation, significant temperature increases and thus a rise in drought frequency [144, 215, 32, 60]. Similar results have been found in northern Italy [12, 129] and southern Italy [186]. However, most of the future projections are based on the SPI/SPEI indices [12, 129, 144, 215] or only precipitation [186, 32].

In this thesis the interest has been in investigating future behaviour of WDI through projections. The analysis focused on the Italian peninsula, which is among the European regions most affected by climate change. Based on the results for the entire country, the analysis was restricted to the Po Valley and Basilicata regions according to the criterion defined in Section 4.3. Figure 5.7 shows the whole Italian territory together with the two selected areas.

Climate projections for the Po Valley region predict a decrease in the number of wet days and an increase in precipitation intensity during storms, resulting in more severe drought conditions, particularly in the Alpine area [12]. These recurring drought conditions are expected to reduce water availability for agriculture, posing a significant challenge for the Po Valley, historically highly devoted to agriculture. The analysis focused on plains identified as areas with elevations lower than 300 metres.

On the other hand, the southern Mediterranean, and especially southern Italy, including Basilicata, appears to be among the regions most affected by precipitation deficits [60].

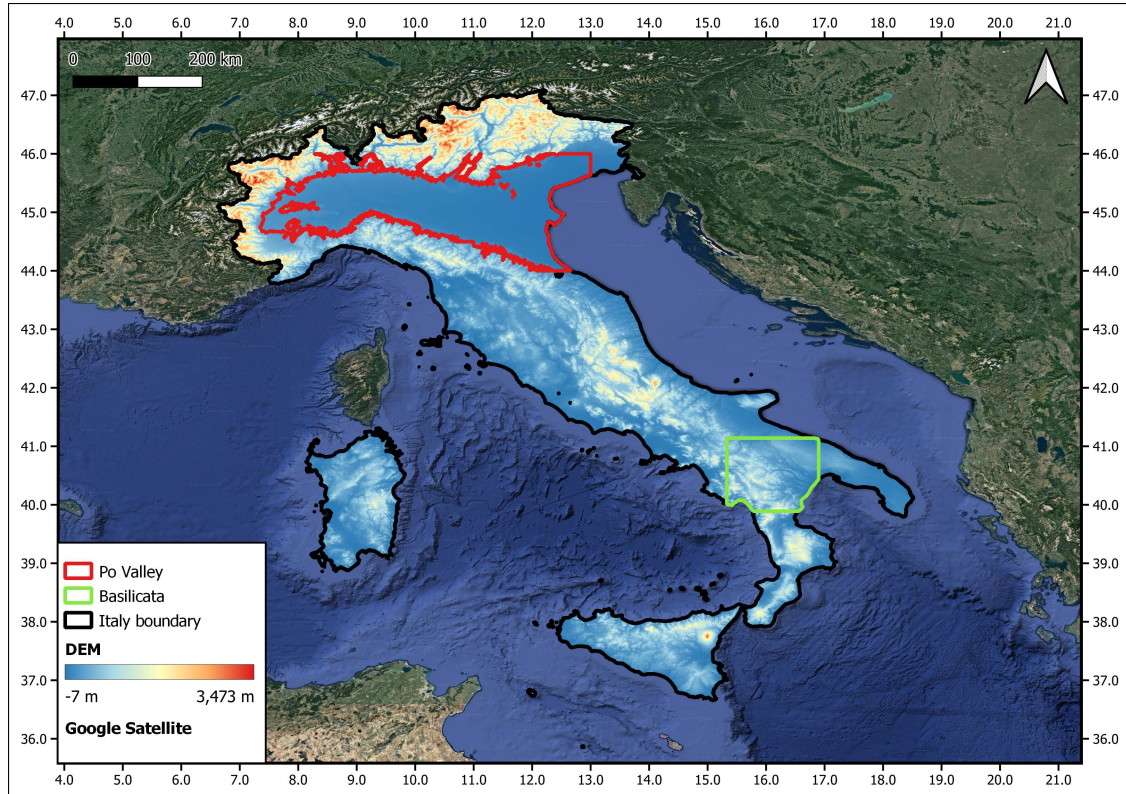


Figure 5.7: The map shows the entire Italian territory, with two selected areas highlighted: the Po Valley plains are shown in red (44–45.5° N, 8–13° E, elevation < 300 m) and the Basilicata region in green (39.89–41.14° N, 15.33–16.9° E). The colour represents altitude (in metres).

5.4.1 Data

To project WDI, regional climate model simulations from the EURO-CORDEX initiative, based on CMIP5 (EUR-11 product), were used. The analysis considered the RCP 4.5 and RCP 8.5 scenarios (future simulations covering 2006–2100) in addition to the historical period (1950–2005). These two scenarios correspond to radiative forcings of 4.5 W/m² and 8.5 W/m², respectively [170, 171]. RCP 4.5 represents an intermediate stabilization scenario, in which greenhouse gas concentrations stabilize after 2050. By maintaining CO₂ concentrations at approximately 543 ppm—nearly double the pre-industrial level of 278 ppm [161]—RCP 4.5 is often considered the most likely trajectory. In contrast, RCP 8.5 depicts a worst-case scenario, characterized by continuously increasing

emissions throughout the 21st century, reaching a radiative forcing of about 8.5 W/m^2 by 2100 and up to 12 W/m^2 by 2250, when concentrations eventually stabilize [161]. Figure 5.8 illustrates the radiative forcing evolution for the four CMIP5 RCP scenarios, which begin to diverge around the year 2050.

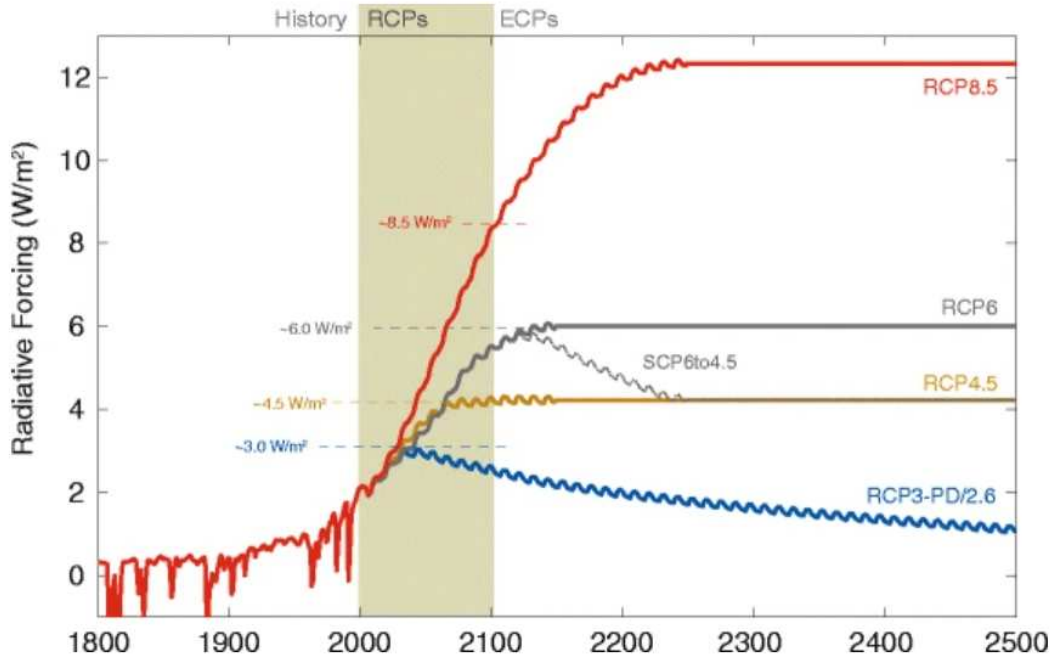


Figure 5.8: Total radiative forcing for the four CMIP5 RCP scenarios: RCP 2.6 (blue), RCP 4.5 (yellow), RCP 6.0 (grey), and RCP 8.5 (red). Short-term variations in radiative forcing are due to both volcanic forcings in the past (1800–2000) and cyclical solar forcing, assuming a constant 11-year solar cycle. Beyond 2100, the scenarios are extended through the Extended Concentration Pathways (ECPs), which provide trajectories up to 2300. Source: Meinshausen *et al.* (2011) [161]

Following the standard CMIP variable naming convention, the model variables used were *ts* (surface temperature), *tas* (2-meter air temperature), and *hurs* (relative humidity). *tas* and *hurs* were used to derive T_d according to Eq. (3.8). The Land Area Fraction (*sft1f* variable in CMIP) was also used to exclude ocean grid cells and restrict the analysis to land surfaces only. However, only a limited number of simulations provide all the necessary variables for both RCPs. Therefore, the analysis was restricted to the 13 simulations listed in Table 5.1. All simulations have a horizontal resolution of 0.11° and a daily temporal resolution.

Unfortunately, following a quality assessment, all models based on the HadGEM2-ES GCM were excluded due to anomalous behaviour affecting both the historical and future periods (e.g., pronounced multi-decadal sinusoidal oscillations and seasonally inconsistent anomalies, with strongly negative winter anomalies in the far-future and positive anomalies in the near-future). This irregular behaviour impacted WDI, LST, and T_d , indicating an upstream issue within those simulations. Consequently, the ensemble was reduced from 13 to 10 members. Further details are

Table 5.1: EURO-CORDEX models used

GCM	RCM	Run	Abbreviation
CNRM-CERFACS-CNRM-CM5	ALADIN63 v2	r1i1p1	CM5-ALAD
CNRM-CERFACS-CNRM-CM5	RCA4 v1	r1i1p1	CM5-RCA4
ICHEC-EC-EARTH	HIRHAM5 v2	r3i1p1	ECE-HIR
ICHEC-EC-EARTH	RACMO22E v1	r1i1p1	ECE-RACM
ICHEC-EC-EARTH	RCA4 v1	r12i1p1	ECE-RCA4
MOHC-HadGEM2-ES	HIRHAM5 v2	r1i1p1	HAD-HIR
MOHC-HadGEM2-ES	RACMO22E v2	r1i1p1	HAD-RACM
MOHC-HadGEM2-ES	RCA4 v1	r1i1p1	HAD-RCA4
IPSL-IPSL-CM5A-MR	RCA4 v1	r1i1p1	IPSL-RCA4
IPSL-IPSL-CM5A-MR	WRF381P v1	r1i1p1	IPSL-WRF
MPI-M-MPI-ESM-LR	RCA4 v1a	r1i1p1	MPI-RCA4
NCC-NorESM1-M	HIRHAM5 v3	r1i1p1	NOR-HIR
NCC-NorESM1-M	REMO2015 v1	r1i1p1	NOR-REMO

provided in Appendix 5.A.

To reduce model uncertainty, particularly in areas characterized by complex topography, an ensemble was created by taking the median across all models, following the approach of [12]. This ensemble approach is essential as it accounts for the the high variability observed not only among different models but also within individual models, where multiple runs can yield slightly different results. All subsequent analyses were conducted at the seasonal scale, with the seasons defined as follows:

- **DJF**: December, January, February
- **MAM**: March, April, May
- **JJA**: June, July, August
- **SON**: September, October, November

5.4.2 Workflow

This section describes the overall workflow used to compute seasonal anomalies (Section 5.4.2); to assess the spatial trends using the Contextual Mann–Kendall (CMK) test on prewhitened time series (Section 5.4.2); to address the multiplicity issue by applying the two-stage False Discovery Rate (FDR) procedure (Section 5.4.2); and to produce representative regional values (Section 5.4.2).

Seasonal Anomalies

To quantify projected climatic variations, anomalies were computed for each scenario (RCP 4.5 and RCP 8.5) and season (DJF, MAM, JJA,SON). These anomalies are relative to a historical baseline (1981-2005), with projections spanning the near-future (2045-2069) and the far-future (2075-2099).

Let $X(s, d, m, y, k)$ denote the daily value of the variable of interest at spatial location s , day d , month m , year y , and for k -th climate model. The ensemble median monthly value $\bar{X}(s, m, y)$ is first calculated as:

$$\bar{X}(s, m, y) = \text{median}_{k=1, \dots, N_{\text{models}}} \left(\frac{1}{N_d(m, y)} \sum_{d=1}^{N_d(m, y)} X(s, d, m, y, k) \right), \quad (5.1)$$

where $N_d(m, y)$ is the number of days in month m of year y and N_{models} is the total number of models considered.

Given a season defined by a set of months $\mathcal{M}$ and a set of years $\mathcal{Y}$ within a given time window (e.g., historical, near-future, or far-future period), the seasonal climatology $\bar{X}(s)$ (mean over months and years) at location s is then calculated as:

$$\bar{X}(s) = \frac{1}{|\mathcal{Y}|} \sum_{y \in \mathcal{Y}} \left(\frac{1}{|\mathcal{M}|} \sum_{m \in \mathcal{M}} \bar{X}(s, m, y) \right). \quad (5.2)$$

Finally, using Eq. (5.2), the seasonal anomalies $\Delta \bar{X}(s)$ were computed as the difference between a future projection (which is either near-future or far-future, denoted by *fut*) and the historical baseline, i.e.

$$\Delta \bar{X}(s) = \bar{X}^{\text{fut}}(s) - \bar{X}^{\text{hist}}(s). \quad (5.3)$$

Trend Analysis

The spatial distribution of WDI, T_s and T_d trends was assessed using the Contextual Mann–Kendall (CMK) test [175]. The CMK test is a modification of the traditional Mann–Kendall (MK) test [148], designed to better characterize geographical phenomena (such as remotely sensed images). Unlike the traditional test, the CMK accounts for spatial autocorrelation by evaluating trends within the local neighborhood of each pixel (a 3×3 neighborhood in this case). The Z -test statistic can be computed as:

$$Z = \frac{\bar{S} - \mathbb{E}[\bar{S}]}{\sqrt{\text{var}(\bar{S})/\sqrt{N_p}}} \quad \text{with} \quad \bar{S} = \frac{1}{N_p} \sum_{j=1}^{N_p} S_j, \quad (5.4)$$

where S_j is Kendall's S for the j^{th} neighbour and $N_p = 9$ pixels, which includes the central pixel and its eight neighbours. Note that $\mathbb{E}[\bar{S}] = 0$ and $\text{var}(\bar{S}) = n(n-1)(2n+5)/18N_p$.

However, an underlying assumption of the MK test family is that data are serially independent, i.e. there is no autocorrelation in the time series. The presence of positive serial correlation increases the probability that the MK tests detect a trend when none actually exists (higher number of Type I errors) [233]. This issue can be addressed either by reducing the effective sample size, by adjusting the variance, or by prewhitening the series to remove serial correlation [175]. Among these methods, prewhitening is the most popular. Prewhitening, first proposed in [233, 206], is the process of fitting time series models, such as autoregressive models, to the original time series and then extracting the residuals to form a new, adjusted time series [194]. Here, the

Variance Corrected Trend Free PreWhitening (VCTFPW) method [238] was applied, utilizing the implementation available in the MATLAB library mannkendall (mannkendall.github.io/Matlab). This method corrects the one proposed in [255] for both the elevated variance of slope estimators and for the decreased slope, and can be summarised as follows:

1. estimate Sen's slope β_{data} from the original series X_t using standard slope estimator;
2. detrend the series, i.e. remove the trend, leaving residuals:

$$A_t^{\text{detr}} = X_t - \beta_{\text{data}} t;$$

3. remove lag-1 autocorrelation a_1^{detr} from A_t^{detr} to produce a detrended prewhitened time series:

$$A_t^{\text{detr-prew}} = A_t^{\text{detr}} - a_1^{\text{detr}} A_{t-1}^{\text{detr}};$$

4. variance correction of the prewhitened residuals. Since prewhitening reduces variance, the variance of the adjusted residuals is restored:

$$A_t^{\text{detr-prew,VC}} = A_t^{\text{detr-prew}} \times \frac{\sigma_X^2}{\sigma_A^2},$$

where σ_A^2 is the variance of the original series X_t , and σ_X^2 is the variance of the prewhitened series $A_t^{\text{detr-prew}}$;

5. correct the slope estimator β_{data} for autocorrelation via the **variance inflation factor (VIF)**:

$$\beta_{\text{VC}} = \frac{\beta_{\text{data}}}{\sqrt{\text{VIF}}} \quad \text{where} \quad \text{VIF} \approx \frac{1 + a_1^{\text{detr}}}{1 - a_1^{\text{detr}}}.$$

- If lag-1 autocorrelation is positive, then $\text{VIF} > 1$ and the slope decreases,
 - if autocorrelation is zero, then $\text{VIF} = 1$ and no adjustment is needed;
6. recombine the variance-corrected detrended-prewhitened time series $A_t^{\text{detr-prew,VC}}$ with the corrected slope β_{VC} to form the VCTFPW-processed series

$$X_t^{\text{VCTFPW}} = A_t^{\text{detr-prew,VC}} + \beta_{\text{VC}} t.$$

In summary, VCTFPW removes the trend (1)-(2), accounts for lag-1 autocorrelation (3), rescales the variance (4), corrects the slope estimate (5), and recombines the series (6). Moreover, cross-correlation was accounted for by introducing an additional covariance term in the variance calculation ([175]) as

$$\text{Var}(\bar{S}) = \frac{1}{N_p^2} \left[\sum_{j=1}^{N_p} \text{Var}(S_j) + 2 \sum_{j=1}^{N_p-1} \sum_{\ell=1}^{N_p-j} \text{Cov}(S_j, S_{j+\ell}) \right].$$

Prewhitening was applied to the seasonal time series spanning 2021 to 2100. Subsequently, the CMK test was performed using the Kenda11 module in TerrSet (clarklabs.org/terrset) at a 95% confidence level. For a given spatial location s , the CMK test was applied to the prewhitened seasonal time series as follows:

$$\text{CMK}(s) = \text{CMK} \left(\text{VCTFPW} \left(\left\{ \frac{1}{|\mathcal{M}|} \sum_{m \in \mathcal{M}} \bar{X}(s, m, y) \right\}_{y=2021}^{2100} \right) \right) \quad (5.5)$$

where $\text{VCTFPW}(\cdot)$ denotes the application of prewhitening to the seasonal time series. The Kendall's τ coefficient from this test measures the direction and strength of the trend: values range from -1 (a perfect negative trend) to 1 (a perfect positive trend), with 0 indicating no significant trend. The p -value associated with this coefficient is also provided. In addition, the Sen's slope (or Theil–Sen estimator) [224] is reported, which quantifies the magnitude of the trend, that is, the average annual change (in this case, °C/year).

False Discovery Rate (FDR) Correction

Care should be taken when interpreting significant trends. In this study, the CMK test was applied across the entire Italian peninsula; however, the resulting map can only suggest potential trends. Drawing conclusions solely based on the significance map would be misleading. Indeed, when working with gridded data, we are performing simultaneous inferences, one for each pixel, so making conclusions about the global significance of the entire field is not appropriate. This issue arises because the significance level does not account for the multiplicity of the tests performed, which can lead to an increased risk of false positives, see [85]. This problem, known as multiple testing or multiplicity, can be addressed by controlling the Family-Wise Error Rate (FWER), for example through the Bonferroni correction [20], or by controlling the False Discovery Rate (FDR) [16]. In the context of gridded data, the FDR control is generally preferred, especially when dealing with hundreds of simultaneous tests, due to spatial dependence [91].

The FDR is the expected proportion of rejected true null hypotheses among all rejected hypotheses. When some of the null hypotheses are false, a procedure that controls the false discovery rate may reject many more such hypotheses compared with the Bonferroni correction, at the cost of a small proportion of erroneous rejections. The Benjamini–Hochberg procedure controls the false discovery rate at a desired level qm_0/m when the test statistics are independent [16] or positively dependent [18] (q is the user-defined desired level (e.g., 0.05), m is the number of hypotheses to test and m_0 is the number of true null hypotheses). Knowledge of m_0 can be very useful for improving the performance of the FDR controlling procedure. For this reason, the two-stage procedure proposed by Benjamini, Krieger, and Yekutieli (2006) [17] for FDR correction was applied in this study.

The idea underlying the two-stage procedure is that the number of true null hypotheses, m_0 , can be estimated from the results of the one-stage procedure. The workflow as described in [17] consists of the following steps:

1. apply the classic Benjamini–Hochberg linear step-up procedure [16] at level $q' = q/(1 + q)$.

Let r_1 be the number of rejected hypotheses. If $r_1 = 0$, do not reject any hypotheses and stop; if $r_1 = m$, reject all m hypotheses and stop; otherwise, continue;

2. estimate the number of true null hypotheses as $\hat{m}_0 = m - r_1$;
3. apply the linear step-up procedure again with the adjusted FDR level $q^* = q'm/\hat{m}_0$.

To assess the significance of trends (q -value < 0.05) over the two target regions depicted in Figure 5.7, the FDR procedure was applied, utilising the MATLAB implementation developed by David Groppe (www.mathworks.com/matlabcentral/fileexchange/27423-two-stage-benjamini-krieger-yekutieli-fdr-procedure).

In [17], the authors proved that when the test statistics are independent, the two-stage procedure controls the false discovery rate at level q . In the case of positively dependent test statistics, if the same set of dependent p -values is used in both stages, it is difficult to study the combined effect analytically, which may cause the false discovery rate in the two-stage procedure to be higher than expected. The simulation study shows that their proposal seems to perform well even in the positive correlated case.

Regional Aggregation

To study the inter-model variability of the WDI, a representative regional value was obtained for each model as follows:

1. definition of the average monthly value $\bar{X}(s, m, y, k)$ for each model as:

$$\bar{X}(s, m, y, k) = \left(\frac{1}{N_d(m, y)} \sum_{d=1}^{N_d(m, y)} X(s, d, m, y, k) \right), \quad (5.6)$$

2. calculation of the seasonal climatology $\bar{X}(s, k)$ (mean over months and years) at location s and for model k as:

$$\bar{X}(s, k) = \frac{1}{|\mathcal{Y}|} \sum_{y \in \mathcal{Y}} \left(\frac{1}{|\mathcal{M}|} \sum_{m \in \mathcal{M}} \bar{X}(s, m, y, k) \right), \quad (5.7)$$

3. finally, for each region $\mathcal{R}$, the values of all included pixels were averaged to obtain the representative regional value as

$$\bar{X}(k) = \frac{1}{|\mathcal{R}|} \sum_{s \in \mathcal{R}} \bar{X}(s, k). \quad (5.8)$$

5.5 Results

Figure 5.9 shows the WDI anomalies of the ensemble for the entire Italian peninsula. For each scenario and season (DJF, MAM, JJA, SON), anomalies were calculated using Eq. (5.3) relative to the historical baseline (1981-2005), with projections shown for the near-future (2045-2069) and

the far-future (2075–2099). For the near-future period (2045–2069), positive WDI anomalies are consistently projected across all of Italy, spanning all seasons and both RCP scenarios. The largest anomalies are observed under RCP 8.5. The highest anomalies are concentrated in the Po Valley, the islands, and the Basilicata region. In the far-future, this spatial pattern persists but becomes more pronounced, reaching up to 2 °C in the worst-case scenario (RCP 8.5). The only exception is winter, when positive anomalies are observed mainly in South Italy, particularly over the islands and the Appennines. Given the widespread and intensifying projected WDI anomalies across the Italian peninsula in the near and far future, it was essential to determine if these changes constitute statistically significant long-term trends over the projection period.

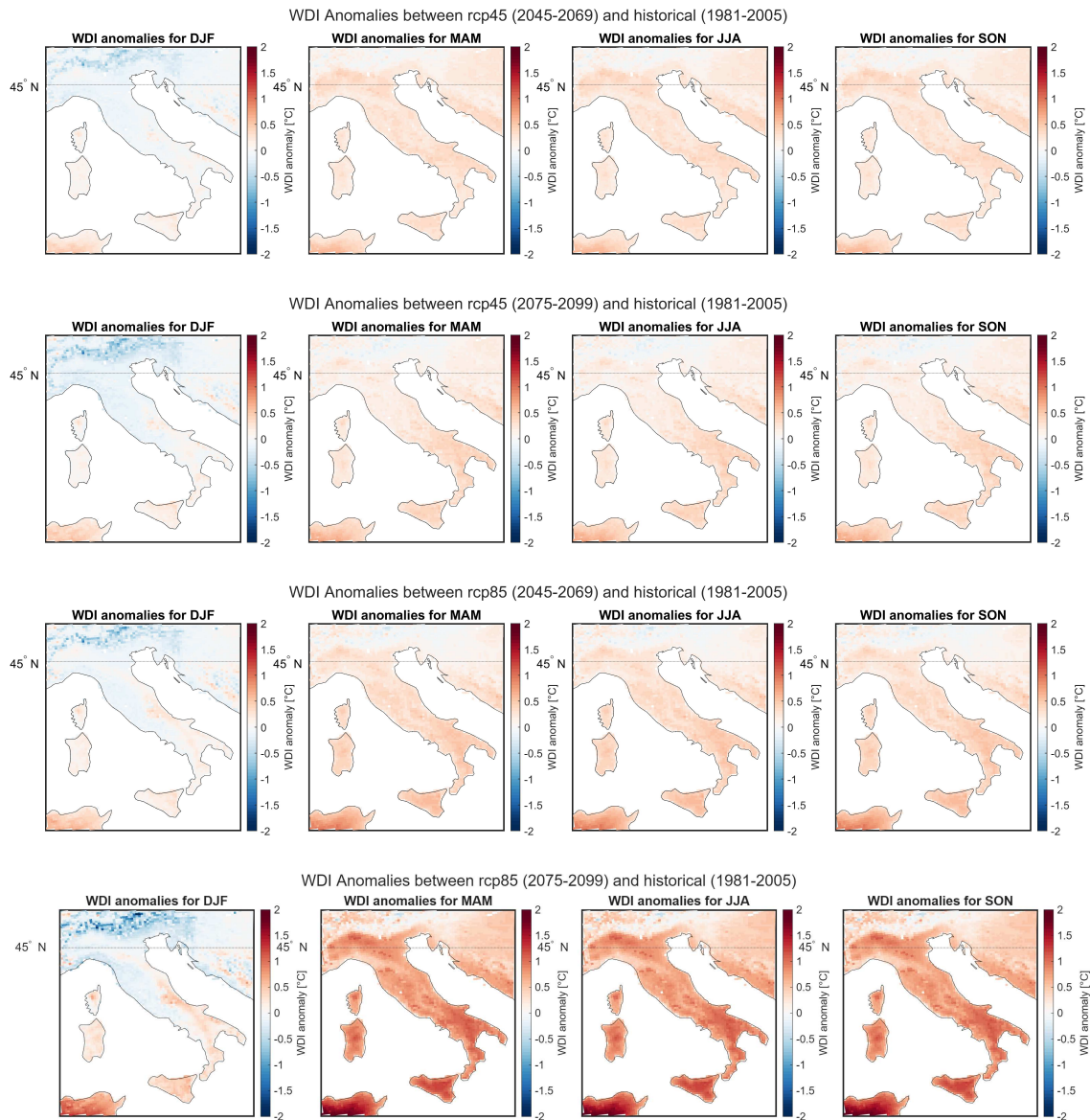


Figure 5.9: WDI anomalies across Italy for each season. First and second row present anomalies for the RCP 4.5 scenario in the near-future and far-future, respectively. Third and fourth row present the same anomalies but for the RCP 8.5 scenario.

A trend analysis of the WDI was subsequently performed using the spatial WDI test at the 95% confidence level, based on seasonal time series from 2021 to 2100 (see Eq. (5.5)). The results under the RCP 4.5 and RCP 8.5 scenarios are presented in Figures 5.10 and 5.11, respectively. Each figure is structured to display:

1. Kendall's τ coefficient (first column);
2. Sen's slope (second column);
3. p -values (third column), where black pixels indicate statistically significant locations (p -value < 0.05).

The WDI trends exhibit mixed results. Under the RCP 4.5 scenario (Figure 5.10), a positive and significant trend is evident in central and southern Italy during winter and, more notably, in spring, with the highest values concentrated in Basilicata and Sicily. In summer and autumn, however, no clear or significant trends are detected. Conversely, under the RCP 8.5 scenario (Figure 5.11) a positive and significant trend is observed almost universally, particularly in Southern Italy and along the Apennine chain. Winter represents an exception, displaying a negative trend in northern and west-central Italy, with the most negative trend centered over the Alps.

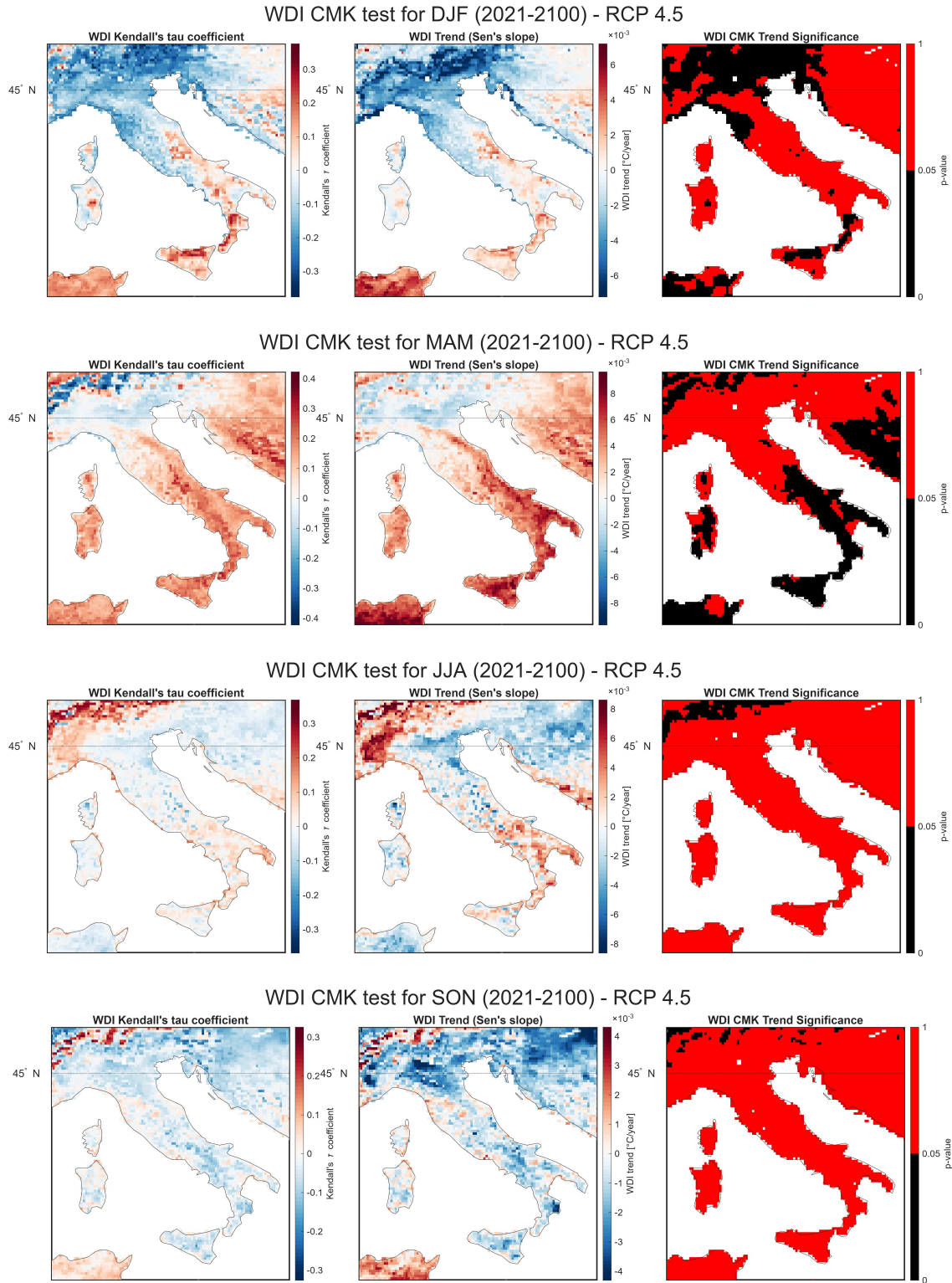


Figure 5.10: CMK test for WDI under the RCP 4.5 scenario. The first column displays Kendall's τ coefficient, the second presents Sen's slope and the third shows the p -value, with black pixels indicating statistically significant locations (p -value < 0.05).

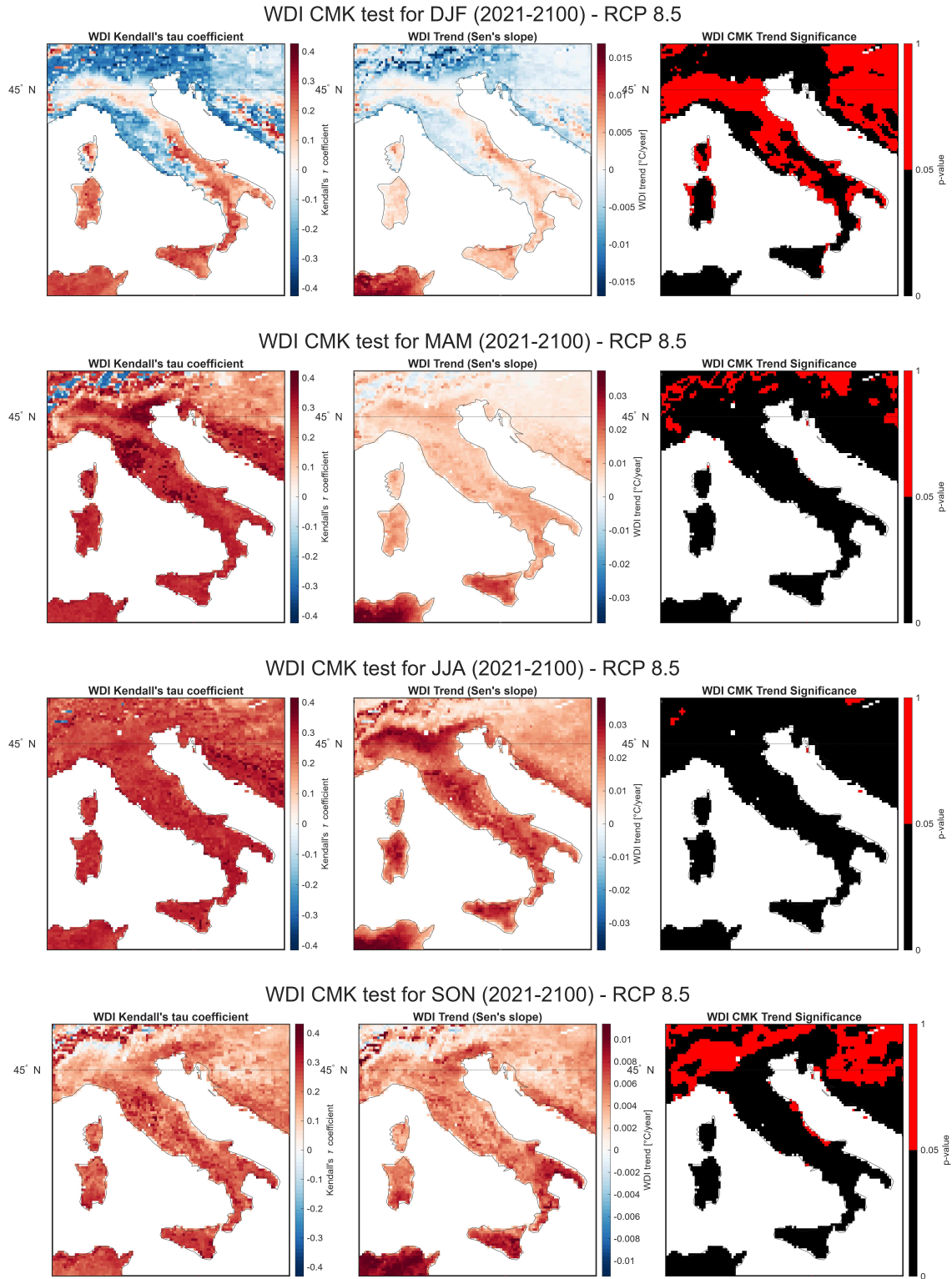


Figure 5.11: CMK test for WDI under the RCP 8.5 scenario. The first column displays Kendall's τ coefficient, the second presents Sen's slope and the third shows the p -value, with black pixels indicating statistically significant locations (p -value < 0.05).

The focus now shifts to the subregions described in Figure 5.7. As previously stated in

Section 5.4.2, the CMK test was computed with the FDR correction applied, which is necessary to draw statistically rigorous conclusions about the trends. Figure 5.12 and 5.13 present the results for the Po Valley, while Figure 5.14 and 5.15 for the Basilicata region. After accounting for multiplicity, it is observed that the trend under the RCP 4.5 scenario in the Po Valley is no longer statistically significant (Figure 5.12). The trend for the RCP 8.5 scenario (Figure 5.13), however, it remains significant in all seasons except winter. Conversely, in the Basilicata region statistical analysis indicates that even under the RCP 4.5 scenario, one season (MAM) exhibits a significant trend, whereas under the RCP 8.5 scenario, the trend is found to be significant across all seasons.

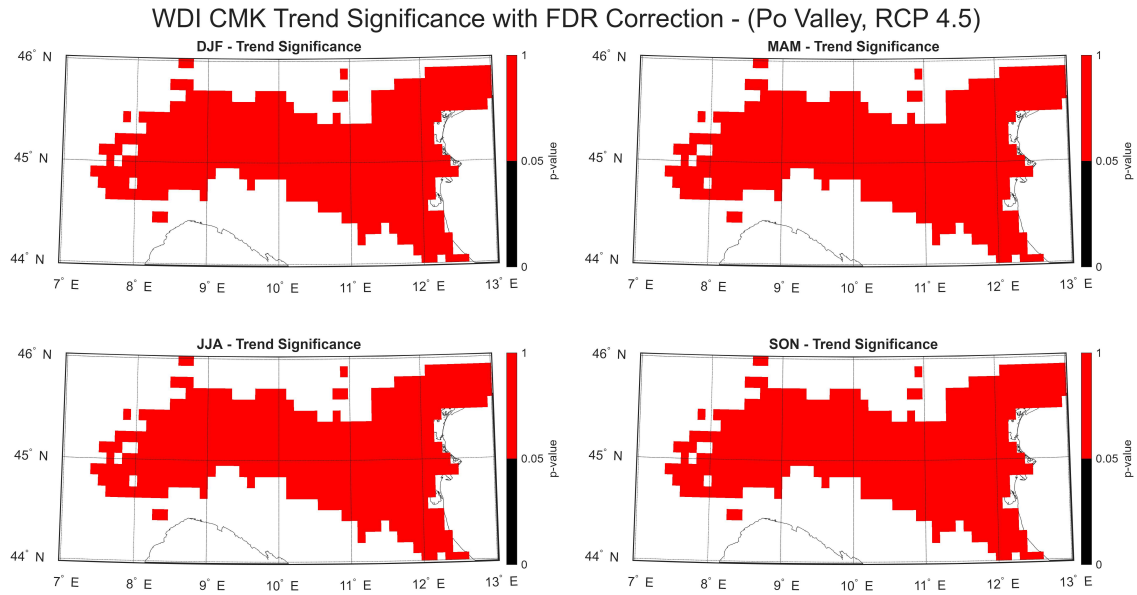


Figure 5.12: CMK trend significance after FDR correction (q -value < 0.05) for the Po Valley under the RCP 4.5 scenario, shown for all seasons.

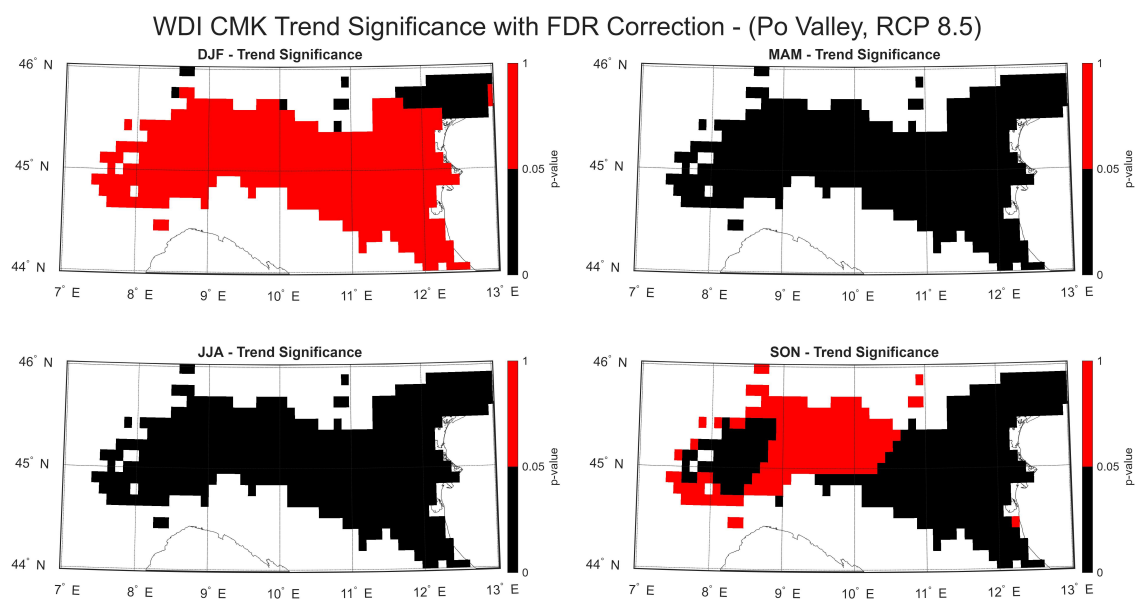


Figure 5.13: CMK trend significance after FDR correction (q -value < 0.05) for the Po Valley under the RCP 8.5 scenario, shown for all seasons.

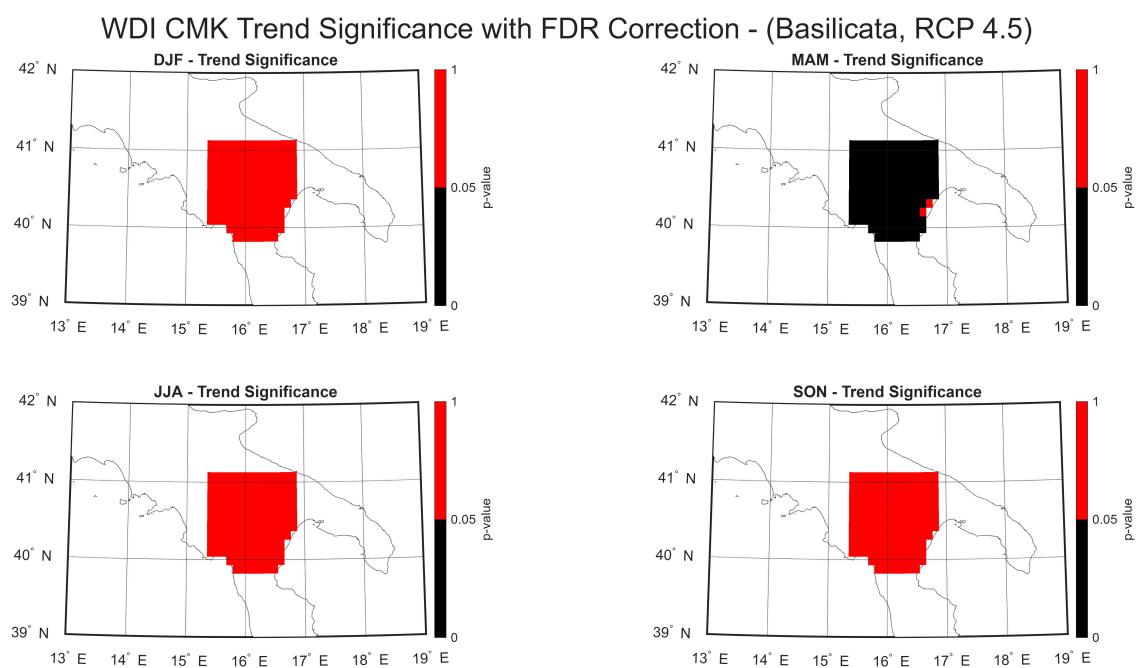


Figure 5.14: CMK trend significance after FDR correction (q -value < 0.05) for the Basilicata region under the RCP 4.5 scenario, shown for all seasons.

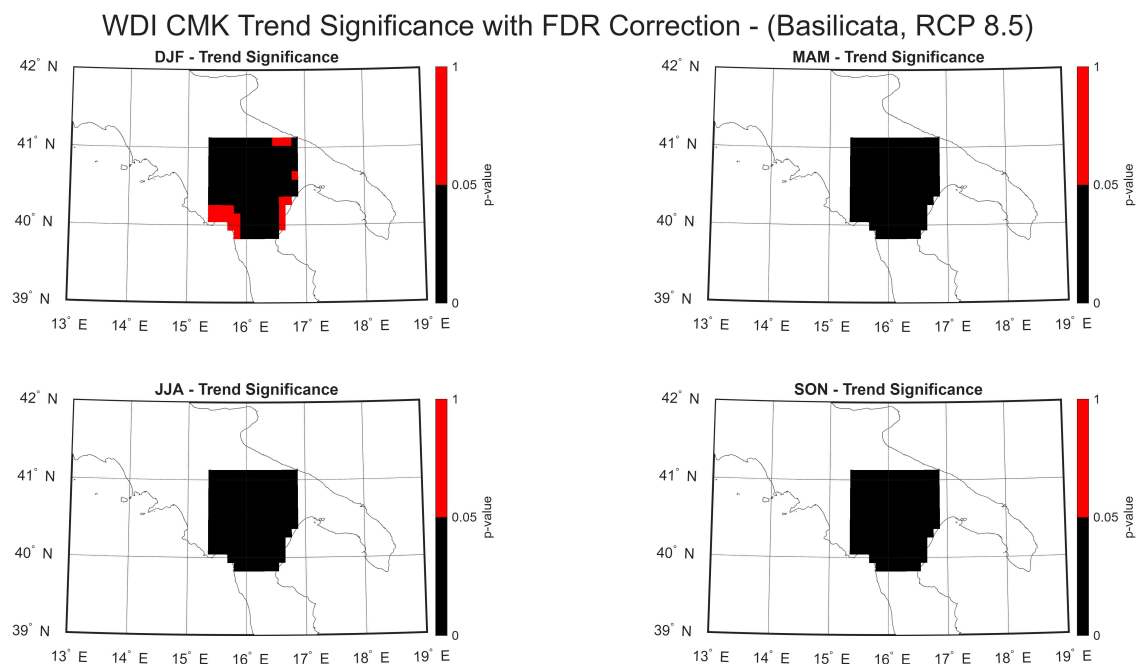


Figure 5.15: CMK trend significance after FDR correction (q -value < 0.05) for the Basilicata region under the RCP 8.5 scenario, shown for all seasons.

Finally, a representative regional value was obtained for each area by averaging the values of all included pixels. This calculation, performed using Eq. (5.8), facilitated the study of both the variability and median trends across the ten climate models utilized.

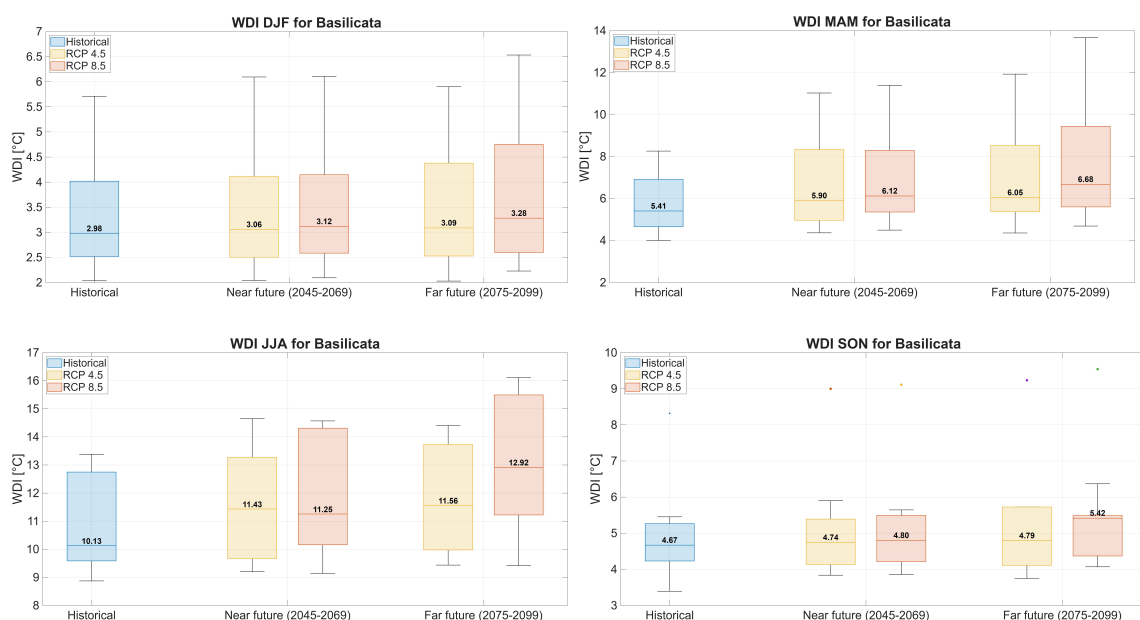


Figure 5.16: Seasonal WDI Boxplot for the Basilicata region under the two scenarios (RCP 4.5 and RCP 8.5).

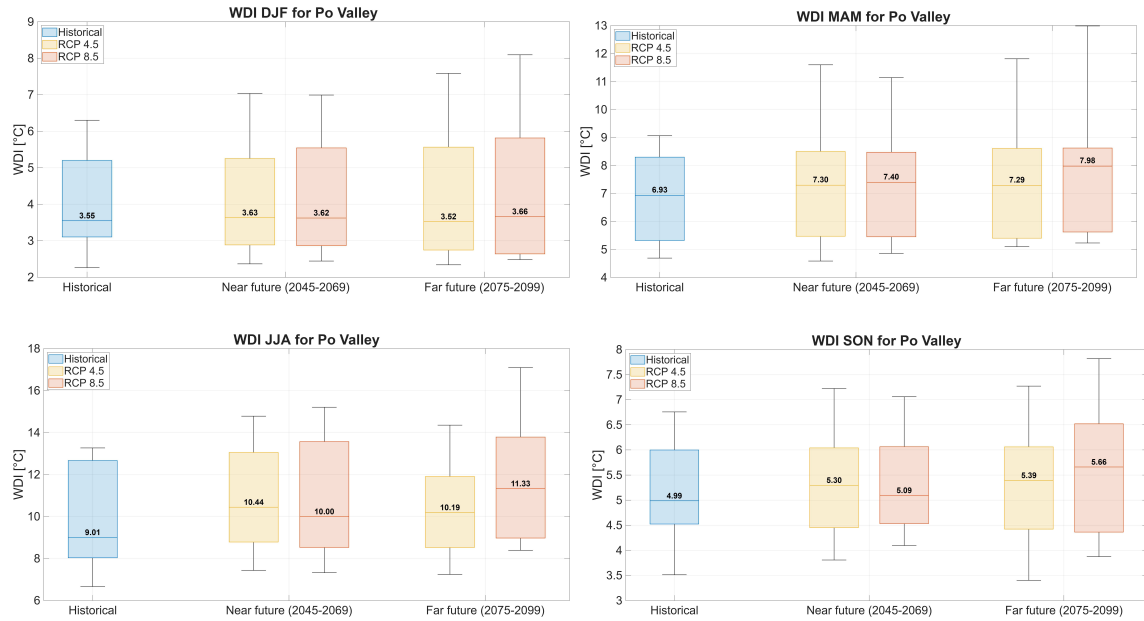


Figure 5.17: Seasonal WDI Boxplot for the Po Valley under the two scenarios (RCP 4.5 and RCP 8.5).

Figures 5.16 and 5.17 illustrate the inter-model variability of WDI for each season and scenario in Basilicata and the Po Valley, respectively. From these boxplots it can be observed that the difference between the two scenarios in the near-future is essentially negligible. An increase in WDI becomes evident only in the far-future, with the largest difference occurring during summer, while differences in the other seasons remain minimal. Among the considered models, the NOR-REMO model occasionally shows WDI values nearly twice as high as those of the other models, particularly in Basilicata during autumn (outliers) and spring (very high upper whiskers).

Figure 5.18 displays the WDI average across all the models at the annual timeframe for each region, illustrating the clear divergence between the two scenarios. In the Po Valley the worst-case scenario (RCP 8.5) begins to diverge after 2060. This difference initiates slightly earlier in the Basilicata region. This pattern is plausible, as the two scenarios have a similar total radiative forcing before 2050 [161], and similar findings have been reported in other studies [66, 113, 180]). The climate system responds relatively slowly to changes in greenhouse gas concentrations due to its large inertia: more than 90% of the excess heat from anthropogenic emissions is stored in the oceans [86], gradually influencing air temperatures. Consequently, even if carbon dioxide emissions were halted immediately, global temperatures would likely continue to rise for decades before reaching equilibrium [254]. This inherent climate inertia makes the choice of RCP scenario particularly relevant only after the mid-century period.

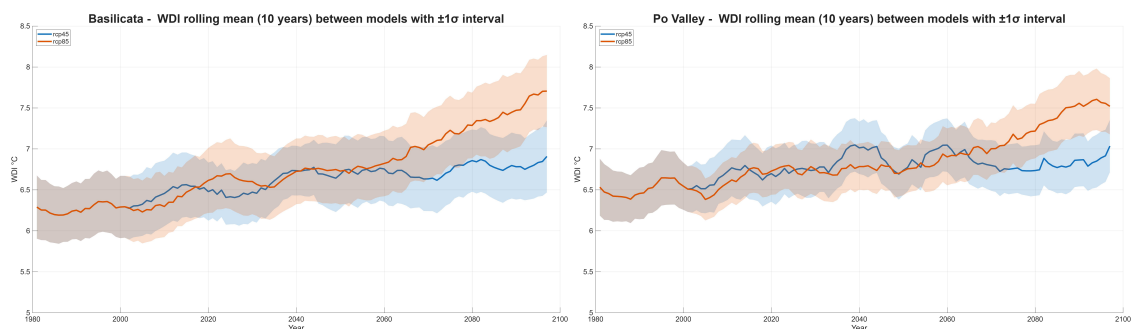


Figure 5.18: Annual WDI average between models (with a 10 years rolling mean) for each region.

For completeness, Figures 5.19 and 5.20 show the seasonal WDI averages across all the models for both regions. A divergence between the two scenarios becomes evident around 2060, particularly in summer, while it remains negligible in winter and autumn.

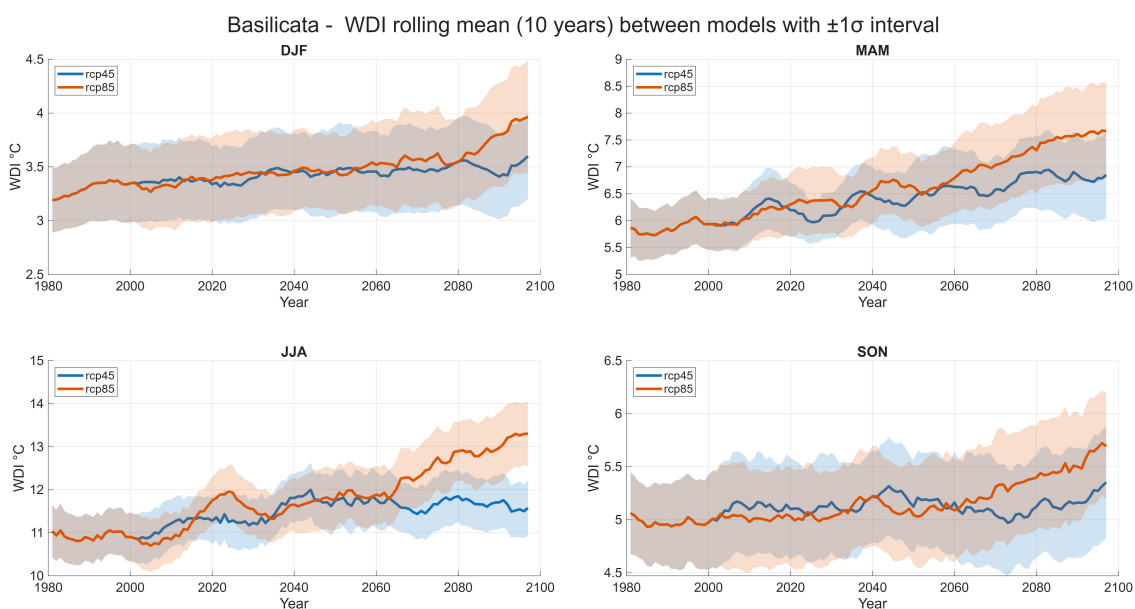


Figure 5.19: Seasonal WDI average between models (with a 10 years rolling mean) for Basilicata.

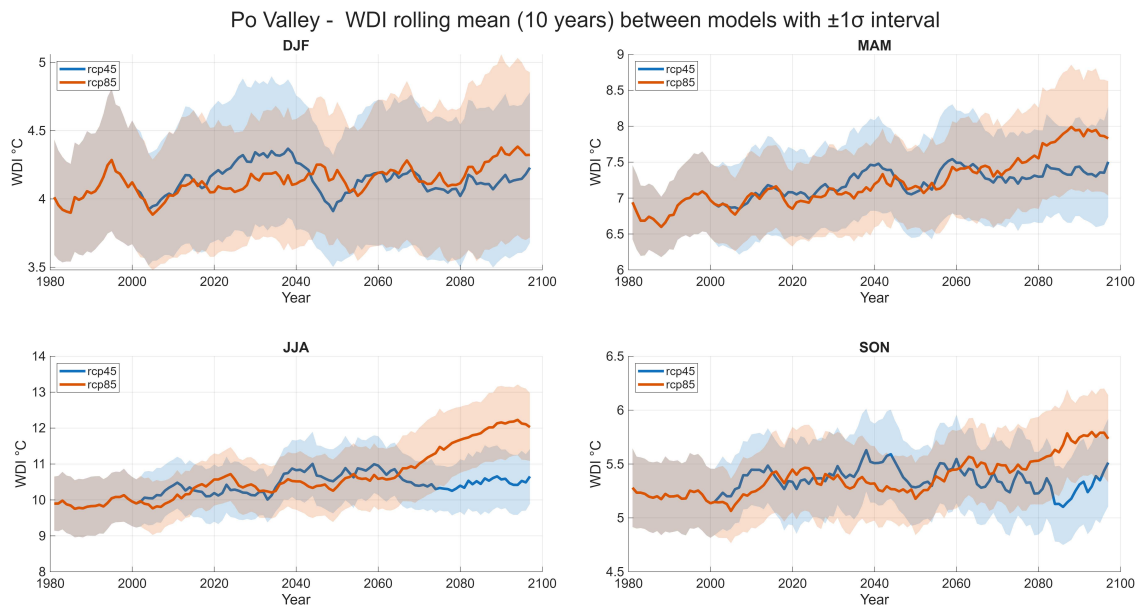


Figure 5.20: Seasonal WDI average between models (with a 10 years rolling mean) for Po Valley.

Appendices

5.A Quality Analysis on HadGEM2-ES GCMs

Following a quality analysis, all models based on the HadGEM2-ES GCM (3 models in total) were excluded. The inclusion of these models resulted in anomalous behaviour, specifically manifesting as highly negative anomalies during winter in the far-future, contrasting with positive anomalies in the near future. This issue was found to affect not only the WDI but also LST and T_d , indicating that the underlying problem resides within the simulations themselves. Figure 5.S1 illustrates the seasonal LST over the Po Valley plains under the RCP 8.5 scenario (a pattern that is also reflected in T_d). A significant disparity is evident between the HadGEM2-ES models and the other models. The HadGEM2-ES models are characterised by a sinusoidal pattern over the years with a periodicity of approximately 60 years. Furthermore, the historical data are also affected, and the timing of the pattern's peaks varies by season. These anomalies tend to cancel out only when averaged across all seasons. For this reason, the number of models utilised in the analyses was reduced from 13 to 10.

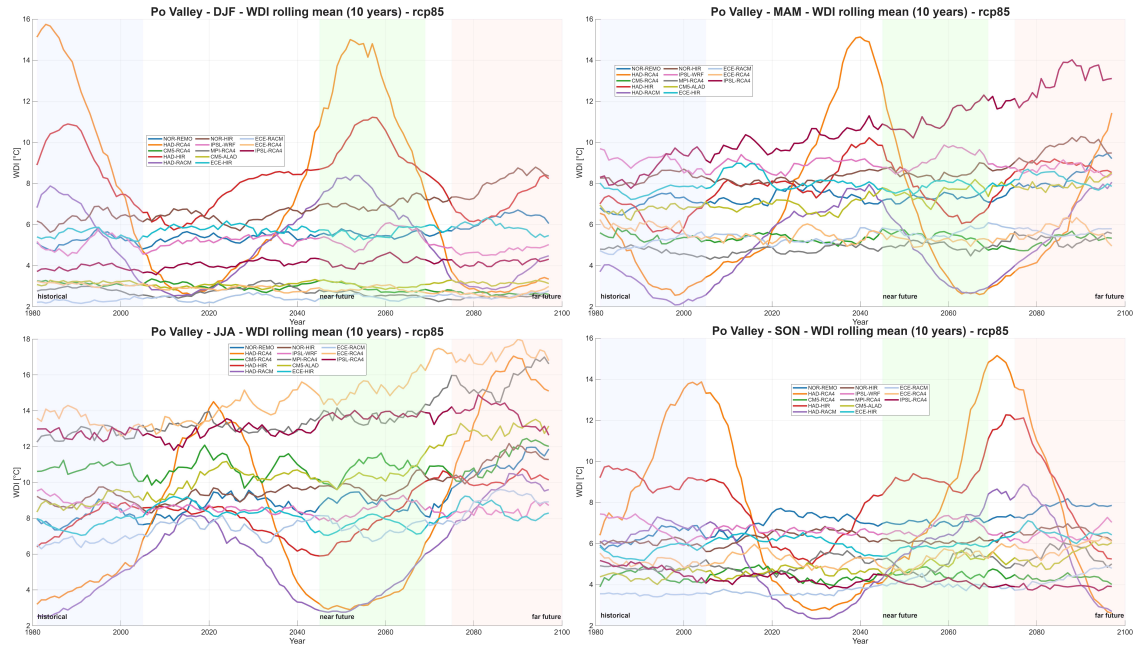


Figure 5.S1: Seasonal T_s over the Po Valley plains under the RCP 8.5 scenario. Each line represents a model, while the blue, green, and red boxes indicate the years used for the historical, near-future, and far-future periods, respectively.



Conclusions and future perspectives

Drought is one of the most complex natural phenomena and among the most difficult to define and monitor, as it develops slowly and often goes unnoticed until its impacts become severe. Vegetation is typically the first systems to exhibit stress due to its high sensitivity to water availability. With the advent of remote sensing, vegetation monitoring has become widely accessible, leading to the development of a wide range of vegetation indices. In this context, a new Water Deficit Index (WDI) was introduced, defined as the linear difference between the LST and the T_d . This index provides a compact and physically interpretable measure of surface heating relative to ambient dryness and has already proven effective in detecting plant water stress. Given that T_d is an atmospheric parameter whose retrieval requires multiple TIR channels, IASI, with its remarkable spectral resolution, was chosen for this purpose. The retrieval of the major atmospheric components, along with LST and T_d , was performed using ϕ -IASI, a FORTRAN-based inverse radiative transfer code designed for the optimal estimation of the thermodynamic state of the atmosphere. The retrieval scheme was tested over two Italian regions: the Po Valley region (northern Italy) and Basilicata region (southern Italy). However, retrievals can be effectively performed only under clear-sky conditions, resulting in sparse and non-homogeneously distributed data over a given spatial domain (L2 observations).

The first objective of this thesis was to develop a robust technique to fill these gaps and produce a gridded product, which was achieved by employing several ML algorithms. The down-scaling–fusion methodology was applied separately to LST and T_d , allowing their independent validation. While the literature contains hundreds of studies on LST downscaling, relatively little attention has been given to IASI-derived LST, whose naturally irregular and scattered observations introduce additional complexity. This is even more true for T_d , whose downscaling has never been addressed before. First, four classical ML algorithms were tested (RF, GBT, NN, and GPR), and GBT exhibited the lowest errors among them. However, the combination of these predictors using Stacked Regression further improved the results. Specifically, the cross-validated MAE and RMSE on the L2 were well below 1 °C for LST and between 2 and 3 °C for T_d . Nighttime overpasses showed the worst results, but this is not a problem since daytime measurements are more relevant for vegetation water-stress monitoring. The generated L3 maps provided a high level of spatial detail, as it was possible to clearly distinguish plains, mountains, and even specific features such as valleys and woodlands. Moreover, this approach was able to retrieve LST and T_d even in months with low IASI L2 density, thanks to the high-resolution spatial covariates used

during the training phase, while maintaining a certain dependence on IASI observations, since only spatial areas with IASI coverage were considered during training. However, a more robust demonstration of the interpolation performance was provided by the validation of both LST and T_d .

The L3 LST was compared with the LST from MODIS, showing strong agreement, with R^2 values greater than 0.90 for almost all months, a standard deviation below 1.5°C , and a bias that fluctuates across months, particularly in the Po Valley, where a clear seasonal bias was observed. This seasonal bias can be explained by the MODIS SW algorithm, which assumes a fixed emissivity, in contrast to our methodology, which simultaneously retrieves both LST and emissivity. The performance of the downscaling method was also assessed by comparing the IASI L2 LST with the colocated MODIS LST. The same seasonal bias and a slightly higher standard deviation persisted, indicating that the differences originate from the products themselves rather than from our downscaling method, which, by contrast, slightly reduced these discrepancies.

Conversely, the L3 T_d was validated against the regional ARPA network, which provides reliable in situ observations across Italy. T_d was computed from the air temperature and relative humidity measured at 2 m by ground stations, and then compared with both IASI L2 and L3 data. The downscaled IASI T_d showed very high agreement with the ARPA stations, with correlation coefficients ranging from 0.87 to 0.94 depending on the overpass time and the target region. These results were very close to those obtained between ERA5 and ARPA. However, it must be noted that ERA5 is a reanalysis product that assimilates ground-based observations, and is therefore expected to perform better than a fully satellite-based dataset. Nevertheless, in the Basilicata region, the L3 T_d correlation was higher than that of ERA5 during daytime, while the bias of the IASI-derived variable remained lower (in absolute value) both during day and night. Interestingly, the bias was consistently positive for both variables in the Po Valley, whereas in Basilicata it was positive only for ERA5 and negative for the IASI T_d . Conversely, the RMSE remained higher for IASI. When also considering the IASI L2 data, the interpolated product showed lower bias, higher correlation, and reduced RMSE, confirming the improvement achieved through the proposed downscaling approach.

The comparison with MODIS for LST and the validation against ARPA stations for T_d showed a better agreement for the L3 product than for the L2, confirming that the enhanced spatial resolution effectively captured the underlying spatial variability. This ensures that the retrieved L3 WDI is also a reliable product, making it possible to test it for detecting plant water deficits. To this end, two homogeneous areas were identified within the two target regions, and for each area a seasonal average was computed for every year to obtain representative WDI values and highlight interannual differences. Comparing these seasonal averages with literature reports showed that the WDI not only successfully captured the years associated with water deficits but also distinguished between years that were both hot and dry and those that were only hot or only dry. For example, in the Po Valley, the WDI showed very high values in 2017 and 2022 but relatively low values in 2024. Indeed, 2024 was hotter than 2017 but much wetter, whereas 2017 was both hot and dry. The ability of the WDI to distinguish between these conditions comes from its two components: LST is highly sensitive to hot surface conditions, while T_d characterises the

atmospheric humidity. For example, the index generally decreases as one approaches coastal areas. This pattern is mainly due to the sea, which increases humidity through evaporation and reduces temperature differences between the land and the air above it. As a result, higher moisture levels cause the index to be consistently lower near the coast. Another example is the Vercelli–Novara plain, where the WDI successfully captured the cooling and humidifying effects of the rice fields, whereas LST and T_d alone fail to do so. Moreover, the higher WDI values along the Appennine chains underscore the importance of detecting plant water stress in the woodlands, where remote sensing is the only viable option for drought monitoring. It is the case of the Basilicata forests, where prolonged drought events have increased tree mortality. All these responses are more difficult to detect using other indices such as the precipitation-based indices, which do not account for the effects of the soil-air interface.

The most severe stress events identified by the WDI were then compared with other remotely sensed water-stress indices, namely the NDMI and SSM. Both SSM and NDMI were consistent with the WDI: high WDI values corresponded to low SSM and NDMI values, indicating that the WDI effectively reflects both soil moisture and vegetation canopy water content. However, this was not always the case: in the Basilicata region, for example, during May and June 2024, the SSM failed to capture the difference between the two months (June was wetter than May), whereas both NDMI and WDI successfully captured this difference. This further confirms the ability of the WDI to detect water stress in plants and its value as a complementary indicator.

Subsequently, the focus shifted toward projecting the WDI using an ensemble of 13 EURO-CORDEX simulations (reduced to 10 after a quality assessment), considering both an intermediate (RCP 4.5) and a worst-case (RCP 8.5) emission scenario. Since many previous studies have mainly focused on precipitation-based indices, this work provides additional value by offering a complementary perspective. The analysis focused on the Italian peninsula and was later restricted to the Po Valley and the Basilicata region. The projections indicated consistent positive WDI anomalies across Italy in all seasons and under both scenarios, suggesting an overall increase in water stress. These anomalies were more pronounced in the Po Valley, the islands, and Basilicata, particularly under the RCP 8.5 scenario, intensifying further in the far future and reaching up to 2 °C in the worst case. Trend analyses revealed predominantly positive and statistically significant trends across Italy and in all seasons under RCP 8.5, with maximum intensity in summer. In contrast, RCP 4.5 showed more localized and less intense statistically significant positive trends. Statistical rigor in the trend analysis was ensured by applying the FDR correction within the two study areas. The Basilicata region is projected to experience a significant WDI increase, potentially worsening tree mortality, particularly in oak forests. In the Po Valley, WDI rises are limited to certain seasons under the worst-case scenario. Divergence between the two scenarios becomes clear only in the far future, especially after 2060, with the largest differences in summer. This lag is due to the climate system's inertia and the similar radiative forcing of the two scenarios before 2050.

The WDI projection results are consistent with those reported in [12], which indicate an intensification of drought severity in the RCP 8.5 scenario, particularly in the far-future. Under

the RCP 4.5 scenario, northern Italy is instead projected to experience increased humidity (i.e., lower WDI values), especially during winter. This finding aligns with [12], which reported that although temperatures in the Po Valley are expected to increase, both scenarios show positive precipitation anomalies in the near future. However, it is important to note that CMIP5 models tend to simulate cooler conditions compared to the newer CMIP6 [41, 259]. In addition, CMIP6 incorporates substantial improvements in the representation of large-scale atmospheric circulation [30] and shows improved skill in capturing the seasonality and intensity of extreme precipitation events [34]. Despite these advances, both CMIP5 and CMIP6 models still exhibit systematic biases. These errors can propagate from GCMs to RCMs degrading the quality of the downscaled simulations [247]. Moreover, downscaling and bias-correction procedures often introduce additional uncertainty, frequently representing a significant source of variability in local climate projections [127], which further complicates analyses at the regional scale. Furthermore, EURO-CORDEX simulations and, in particular, RCMs, do not accurately reproduce observed drought changes [129, 187]. This suggests that future drought trends may be underestimated, and consequently, projections based on these models should therefore be interpreted with caution. Nevertheless, future studies could benefit from the integration of CMIP6 datasets within the CORDEX framework, which provide improved physical representations and updated emission scenarios. In conclusion, the analysis indicates that climate trends may worsen soil erosion, vegetation stress, and water scarcity. In the intensively cultivated Po Valley, increasing water deficits will require new irrigation resources. In southern Italian forests, higher water stress accelerates ongoing dieback and raises wildfire risks. Currently, WDI can be used to monitor large forested areas for these risks and to evaluate mitigation strategies in regions where natural and human-managed ecosystems are particularly vulnerable to climate change.

The greatest advantage of this work lies in the generation of high-resolution and gap-free LST and T_d fields from IASI. The validation of these variables confirmed the quality of the downscaling–fusion methodology proposed here. These two variables were then used to generate high-resolution maps of the WDI, an index shown to be strongly correlated with plant water stress and potentially valuable for drought monitoring. In the future, by processing additional years, it will also be possible to compute WDI anomalies relative to a baseline. This will provide a simpler perspective on the onset of drought events and help identify areas particularly vulnerable to drought conditions, such as the Basilicata region, which is projected to be among the most affected areas.

Furthermore, this study was carried out in the perspective of the new missions IASI Next Generation (IASI-NG) onboard the MetOp Second Generation (Metop-SG) satellite, and the Infrared Sounder (IRS) onboard the new Meteosat Third Generation Sounder (MTG-S) satellite. The IASI-NG instrument, launched in August 2025, is characterized by a spectral resolution that is twice as high as that of IASI. The complex retrieval algorithm developed for IASI, together with the downscaling approach proposed in this work, can be extended to IASI-NG in a straightforward manner. The IRS, launched in July 2025, is a Fourier transform infrared spectrometer belonging to the same instrument class as IASI. On the other hand, the IRS is the first hyperspectral infrared

interferometer on a geostationary satellite providing full-disk coverage. Its spectral coverage, although more limited than that of IASI, consists of two bands: one in the longwave spectral region (679 to 1210 cm^{-1}) and the other in the mid-infrared (1600 to 2250 cm^{-1}), for a total of 1953 channels [64]. However, since IRS operates from a geostationary orbit, it will perform measurements every 30 minutes with a spatial resolution of 4 km at nadir, thereby enabling a better temporal tracking of surface and atmospheric processes.

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