

Inferring the relationship between soil temperature and the normalized difference vegetation index with machine learning

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ABSTRACT

Changes in climate can greatly affect the phenology of plants, which can have important feedback effects, such as altering the carbon cycle. These phenological feedback effects are often induced by a shift in the start or end dates of the growing season of plants. The normalized difference vegetation index (NDVI) serves as a straightforward indicator for assessing the presence of green vegetation and can also provide an estimation of the plants' growing season. In this study, we investigated the effect of soil temperature on the timing of the start of the season (SOS), timing of the peak of the season (POS), and the maximum annual NDVI value (PEAK) in subarctic grassland ecosystems between 2014 and 2019. We also explored the impact of other meteorological variables, including air temperature, precipitation, and irradiance, on the inter-annual variation in vegetation phenology. Using machine learning (ML) techniques and SHapley Additive exPlanations (SHAP) values, we analyzed the relative importance and contribution of each variable to the phenological predictions. Our results reveal a significant relationship between soil temperature and SOS and POS, indicating that higher soil temperatures lead to an earlier start and peak of the growing season. However, the Peak NDVI values showed just a slight increase with higher soil temperatures. The analysis of other meteorological variables demonstrated their impacts on the inter-annual variation of the vegetation phenology. Ultimately, this study contributes to our knowledge of the relationships between soil temperature, meteorological variables, and vegetation phenology, providing valuable insights for predicting vegetation phenology characteristics and managing subarctic grasslands in the face of climate change. Additionally, this work provides a solid foundation for future ML-based vegetation phenology studies.

1. Introduction

In-situ monitoring of changes in vegetation in inaccessible Arctic regions is challenging, prompting many such studies to rely on remote sensing techniques (Zmarz et al., 2018). In the field of remote sensing, vegetation indices such as the Normalized Difference Vegetation Index (NDVI) are used to quantify and qualify vegetation cover (Huang et al., 2021). This is achieved through airborne or satellite spectral methods (Ryu et al., 2021; Zhao et al., 2021) or ground-level measurements,

using handheld instruments (Balzarolo et al., 2011; Ferrara et al., 2010). Vegetation activity monitoring using NDVI has shown both intra-annual and inter-annual variations that can give valuable insights into ecosystem changes (Beck et al., 2006; Rhif et al., 2022). Some parameters that can be derived from such intra-annual seasonal NDVI curves are the start of the season (SOS), peak of the season (POS), and maximum annual NDVI value (PEAK) (Li et al., 2017; Ma et al., 2022).

In high latitudes, the intra-annual temperature and irradiance variation are important factors that control the cycles in the growth and

Abbreviations: NDVI, Normalized Difference Vegetation Index; SOS, start of the season; PEAK, maximum annual NDVI value; POS, peak of the season; ML, machine learning; ANN, artificial neural network; MLP, multilayer perceptron; MSE, mean squared error; MAE, mean average error; CV, cross validation; SHAP, SHapley Additive exPlanations; LIME, Local Interpretable Model-Agnostic Explanations; xAI, explainable artificial intelligence.

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reproduction of the flora (Møllmann et al., 2021; Odland et al., 2003). Over the last decades, different life-cycle events of vegetation (phenology) have been observed to change in this region (Epstein et al., 2013). This has been related to ongoing climate change (IPCC, 2021), which has started to affect vegetation phenological cycles, productivity, and community structure (Semenchuk et al., 2016). Inter-annual analyses found relationships between climate change and these changes in vegetation dynamics, particularly with regard to the increase in surface temperature, resulting in an increased PEAK NDVI and with a notable impact on the length of the growing seasons (Arndt et al., 2019; Potter and Alexander, 2020). Starting from the year 2000, scientists started to name this phenomenon of an increasing PEAK “Arctic greening” (Merrington, 2019). This phenomenon was hypothesized to persist with continued climate warming, based on the compelling evidence of increased PEAK NDVI (Beck and Goetz, 2011), plant productivity (Lorant and Goetz, 2012), phenology (Semenchuk et al., 2016), and vegetation composition (Walker et al., 2012b) between 1980s and early 2000s (Epstein et al., 2012, 2013).

Interestingly, the “Arctic greening” effect has not occurred everywhere at high latitudes and since the early 2000s, the relationship between PEAK NDVI with an increase in surface temperature has weakened in many places (Bhatt et al., 2013; Myers-Smith et al., 2020). In fact, in some regions, this relationship has even become negative, introducing the term “Arctic browning” (Beck and Goetz, 2011). It is generally believed that the shift towards browning must indicate that other meteorological drivers (e.g., temperature, precipitation, wind, photoperiod) or biological drivers (e.g., insect grazing, drought, etc.) are in play. However, the issue still requires further study.

In Iceland, the same strong “Arctic greening” trend was shown to occur during the 1980s–2000s as in many other high-latitude regions, but with a notable stagnation of the national PEAK NDVI during 2000–2010, even if the surface temperatures continued to increase in Iceland during that period (Björnsson et al., 2007; Raynolds et al., 2015). What happened in Iceland after 2010 is unclear, but a recent study showed that the inter-annual variation in the national average PEAK NDVI has been large during 2001–2019 period (Olafsson and Rousta, 2021). Therefore, it is of interest to further study how the NDVI of Icelandic ecosystems responds to further warming.

The impact of climate change on high latitude vegetation is not only limited to the air temperature increases. Soil warming studies have revealed significant insights into how soil warming affects soil processes and, consequently, vegetation. Soil warming experiments in high latitudes have demonstrated that increased soil temperatures can lead to changes in nutrient availability, microbial activity, plant composition and biomass, all of which influence plant growth and ecosystem dynamics (Fang et al., 2023; Metze et al., 2024; Verbrugghe et al., 2022b). For example, Bhattarai et al. (2023) found that soil warming resulted in changes to below-ground plant biomass and fine root biomass, under different warming conditions. These changes were associated with shifts in plant community composition and soil chemistry, highlighting the complex adaptation mechanisms of subarctic grasslands to prolonged soil warming.

Continued climate change is expected to cause relatively higher increases in surface temperatures at higher latitudes in the coming decades (IPCC, 2021), which will likely lead to relatively more ecosystem changes in plant productivity than at lower latitudes (Chen et al., 2021). Potential changes include further temporal shifts in parameters that characterize growing seasons (Semenchuk et al., 2016) and increases in plant productivity (Street and Caldararu, 2022; Van Der Wal and Stien, 2014). However, it is important to further investigate the warming impacts on NDVI to better underpin such predictions for future changes. Combining data from manipulation (warming) experiments offer possibilities to study future high-latitude ecosystem NDVI responses (Bjorkman et al., 2020; Leblans et al., 2017).

To relate changes in vegetation composition, biomass or NDVI to environmental parameters, traditional statistical methods like (non-)

linear regression or linear mixed models have been most commonly used (Estrella et al., 2021; Hope et al., 1993; Leblans et al., 2017; Mehmood et al., 2024; Walker et al., 2012a; Wang et al., 2021). Additionally, multivariate methods have also been used, for example multivariate analysis of variance tests (Michielsen, 2014).

Despite massive advancements in the field of machine learning (ML) during the last decade, ML is not yet often used for vegetation studies. ML models can be used for various tasks, among which are classification, regression, and image segmentation. In ML, models extract knowledge from data and use this knowledge to produce an output relevant to the task at hand. These models use three main learning paradigms: supervised learning, unsupervised learning or reinforcement learning. This study only considers the first paradigm, as we build a regression model. Within supervised learning, there are a multitude of model types, for example, support vector machines (Hearst et al., 1998), boosted tree ensembles (e.g., XGBoost (Chen and Guestrin, 2016) or LightGBM (Ke et al., 2017)) and artificial neural networks (ANNs) (McCulloch and Pitts, 1943). This analysis will use ANNs, particularly multilayer perceptrons (MLPs), which are fully connected feedforward neural networks that consist of multiple layers of nodes that are connected with each other by weighted edges.

Recently, ML has also shown promising results in the field of ecology (Christin et al., 2019; Thessen, 2016), for use cases such as species identification (Barhate et al., 2023; Barré et al., 2017; Chen et al., 2020; Wäldchen and Mäder, 2018), behavioral studies (Clapham et al., 2020; Schofield et al., 2019), ecological modeling and forecasting (Cho et al., 2009; Strydom et al., 2021; Ye and Cai, 2011), remote sensing (Guo et al., 2020; Li et al., 2020) and climate change studies (Kumar, 2023; O’Gorman and Dwyer, 2018; Rolnick et al., 2022), among others. The utilization of ML techniques has opened new avenues for understanding complex ecological phenomena and predicting ecological responses. Considering the proven potential of ML in addressing research questions in the broad field of ecology (Gao et al., 2024; Jemeljanova et al., 2024), we propose to apply ML methods to investigate the relationship between vegetation phenology and environmental drivers in subarctic grasslands.

Unfortunately, MLPs are black-box models. This means that, while they can approximate any function, it is nearly impossible to determine the structure of the approximated function. This led to a whole new field within ML, explainable artificial intelligence (xAI), which tries to create methods that allow human users to understand the predictions made by an ML model (Vilone and Longo, 2021). Some popular examples include sensitivity analysis (Zeiler and Fergus, 2014), Local Interpretable Model-Agnostic Explanations (LIME) (Ribeiro et al., 2016), and SHapley Additive exPlanations (SHAP) values (Lundberg et al., 2017). This study uses the last method, as it is gaining in popularity and is now often used in ecology. For example, Masago and Lian (2022) use SHAP values to investigate how inter-annual variation in the daily average temperature affected the first flowering date or the full blossom date of the Yoshino cherry trees in Japan. He et al. (2022) construct a seagrass distribution model and explain the importance of environmental variables in the model and subsequent predictions. In Park et al. (2022), an XGBoost model is trained to predict chlorophyll concentration, and they use SHAP values to perform feature selection, as well as investigate feature importance. SHAP values have a number of advantages over other methods for understanding the output of a model. First, SHAP values are model-agnostic, which means that they can be used with any ML model (Lundberg et al., 2017). Second, SHAP values are able to account for interactions between features, which is something other methods are not able to do. Third, SHAP values have an intuitive interpretation, which means that they are easy to understand and explain to others. Finally, SHAP values have some desirable mathematical properties, such as local accuracy, missingness, and consistency (Aas et al., 2021).

An earlier study was conducted by Leblans et al. (2017) at the same research sites in Iceland (Sigurdsson et al., 2016), focusing on the phenology of subarctic grasslands. They used a short-term temporal

dataset from 2013 to 2015 with curve function fitting analyses based on the methodology proposed by Zhang et al. (2003) to determine seasonal (intra-annual) parameters (e.g. SOS). They found that the response towards earlier SOS in the warmed subarctic grasslands did not saturate at higher soil warming levels (i.e., +10 °C). Therefore they concluded that growing seasons at high-latitudes grasslands are likely to continue lengthening with future warming. However, there was still quite a large unexplained inter-annual variability in their 3-year dataset, that warranted a further study (Leblans et al., 2017). In this study, we extended the analysis period to six years, compared to the three years used by Leblans et al. (2017). This enabled a more comprehensive examination of the inter-annual variability in NDVI phenology and annual maximum values. Specifically, the variables used to study NDVI phenology were the annual day numbers of the SOS and POS, as well as the PEAK, in each plot. Our primary objective was to reanalyze the soil warming effects using conventional linear statistics, as performed by Leblans et al. (2017), and to assess the robustness of these relationships over a longer timeframe. Additionally, our study extends previous research by employing ML algorithms to identify further drivers of the unexplained inter-annual variation in the studied variables. Specifically, we added a set of three meteorological variables, namely air temperature, precipitation, and irradiance. However, as predictions made by ML are often not intuitive, we used xAI methods, providing deeper insights into the model outputs.

Our objective was to study the relationship between soil temperature and vegetation phenology. More specifically, we studied this relationship using three vegetation phenology characteristics: SOS, POS and PEAK. Additionally, we investigated the effect of other meteorological variables on these characteristics. To this end, we postulated following hypotheses:

A Soil warming

- i. A higher soil temperature will introduce significantly earlier SOS, as was found by Leblans et al. (2017) for individual years.
- ii. The POS will take place at a similar time each year, regardless of the soil temperature. Plants must use some external trigger to “know” when to start to slow down growth and prepare for autumn. The prevailing theory suggests that for most plants, this is triggered by the length of the day (Adams and Langton, 2005; Roeber et al., 2022), which remains consistent across different years, and is mediated through the phytochrome system (Sigurdsson, 2001).
- iii. The PEAK value will not be significantly related to soil temperature, as Verbrugghe et al. (2022a) showed that there was no difference in above-ground biomass between the warming treatments.

B Other meteorological variables

We expect that ML can identify other important controls for the previously observed inter-annual variability of NDVI phenology and PEAK values. Additionally, we expect that ML can identify the importance of meteorological variables compared to the soil temperature. Out of the three additional meteorological variables, we hypothesized for both phenology and PEAK values:

- i. Larger impact of meteorological variables compared to the soil temperature, as they can also impact the soil temperature (Beer et al., 2018; Tan et al., 2022; Xie et al., 2021).
- ii. Within the meteorological variables, air temperature's influence is expected to be the smallest due to its regulation of soil temperature, while precipitation may have an intermediate effect given consistently high soil water content in these areas (Sigurdsson et al., 2016). Additionally, a substantial impact of irradiance is hypothesized, particularly in consistently cloudy sub-Arctic climates (Hou et al., 2015).

Ultimately, the contributions of this research advance our understanding of the relationships between soil temperature, other

meteorological variables, and vegetation phenology. We achieve this goal by employing a methodology that exceeds standard practice, using ML and SHAP values.

2. Materials and methods

2.1. Data

The study was carried out in the south of Iceland near the village of Hveragerdi on the ForHot site (Sigurdsson et al., 2016), as shown in Fig. 1. Following an earthquake in May 2008, the bedrock of one unmanaged (cold) grassland field site underwent a disruption, resulting in the creation of areas with differently warmed soils. Another nearby grassland field site had had such warmed soil gradients for at least six decades, and those were not disturbed by the earthquake in 2008 (Sigurdsson et al., 2016). In spring 2013, five transects were selected in each field site, each with five permanent plots across the natural soil temperature gradients, resulting in a total of 50 studied plots. We categorized the plots according to their annual soil temperature range, as indicated in Table 1.

2.1.1. NDVI data

To be able to estimate vegetation phenology characteristics, we measured the NDVI of all studies plots using a handheld instrument from SKYE Instruments (SpectraoSense2). From 2014 to 2019, NDVI measurements were done approximately bi-weekly from April to November, except during periods with continuous snow cover in early spring, late autumn, or winter. The measurements were always conducted on a clear day. We refer to Leblans et al. (2017) for further information about the NDVI measurements. As can be seen in Fig. 2, the NDVI data clearly

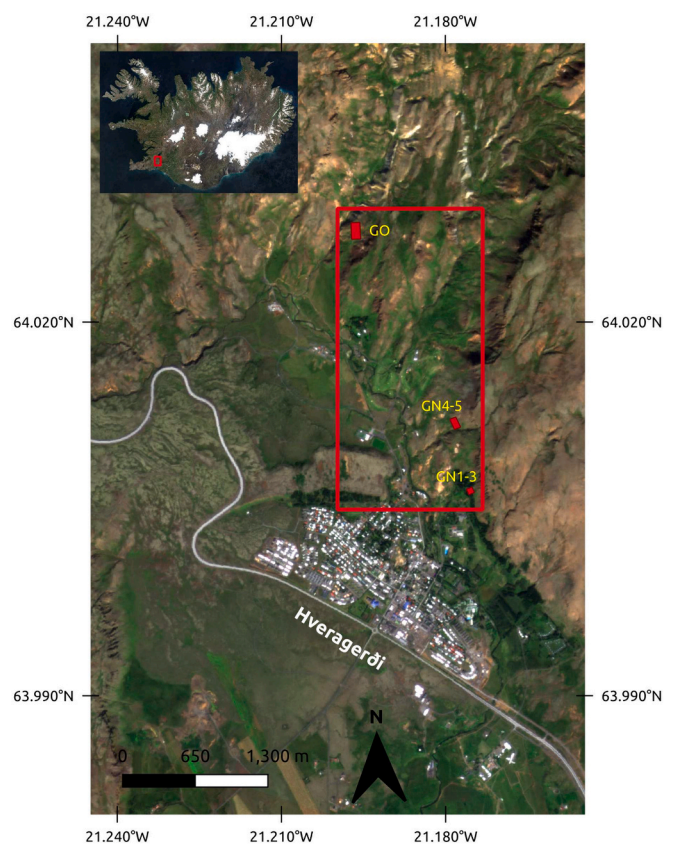


Fig. 1. Map depicting the research site locations near the village of Hveragerdi, Iceland. “GO” (grassland old) marks the sites where the soil has been warming for over six decades, and “GN” (grassland new) denotes the sites where soil warming began following the May 2008 earthquake.

Table 1
Category of the temperature range of the plots.

Category	Temperature Range
A	Ambient
B	+0.5 to 1 °C
C	+2 to 3 °C
D	+3 to 5 °C
E	+5 to 10 °C

2.2. Data analysis

2.2.1. Estimating the NDVI seasonal characteristics

To extract the intra-annual vegetation phenology characteristics (SOS, POS and PEAK) in each plot during each growing season, we first fitted a curve to the measured NDVI data. Based on the approach of Zhang et al. (2003), we used a double logistic curve. We require that the two logistic curves transition into each other continu-

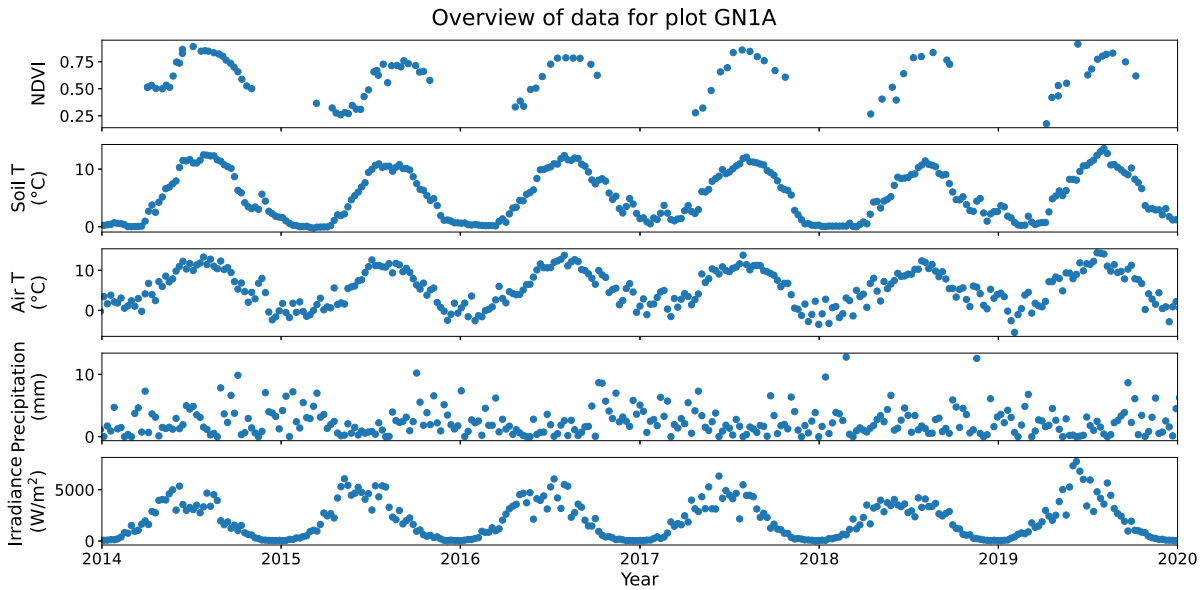


Fig. 2. Overview of all available variables for plot GN1A (unwarmed control plot). Whereas the NDVI and soil temperature (upper two figures) are unique for all 50 plots, the meteorological variables (bottom three figures) are the same for every plot.

showed a seasonal pattern, with a higher NDVI in the summer months.

2.1.2. Soil temperature data

The soil temperature at a depth of 10 cm was monitored in all the permanent plots using HOBO TidbiT v2 Water Temperature Data Loggers (Onset Computer Corporation, USA) since the spring of 2013 (Sigurdsson et al., 2016). In Table 1, the different soil warming categories with their accompanying temperature range are given, while Fig. 2 shows the data for one of the 50 plots used in this study. The main soil warming effect was an approximately constant shift in temperature across the seasons, as shown by Sigurdsson et al. (2016).

2.1.3. Meteorological data

In addition to NDVI and soil temperature data, we also used meteorological data. As the measurement of meteorological variables such as irradiance (global radiation), precipitation, and air temperature at the Forhot site only began in 2019, we relied on data from another source. Specifically, we obtained the aforementioned meteorological variables from a weather station in Reykjavík,¹ located approximately 40 km from the research site, as this is the closest station where irradiance is measured. We aggregated the data by taking the average on a weekly resolution scale, and assumed that the weather conditions are the same for all plots during each year. Given the distance between the weather station and the research plots, the data serve as a proxy for the actual weather conditions at the ForHot site. In Fig. 2, the three bottom panes show all meteorological variables measured in the relevant period.

ously, such that the resulting function is differentiable at every point. These requirements result in the following formula for the estimated NDVI:

$$\widehat{NDVI}(x) = \begin{cases} \frac{c}{1 + e^{b_1 \cdot (x - a_1)}} + d & x \leq p \\ -\frac{c}{1 + e^{b_2 \cdot (x - a_2)}} + d + c & x > p \end{cases} \quad (1)$$

where the parameters a_1 , a_2 , b_1 , b_2 , c , d and p are fitted to a season's NDVI data and x represents the week number ($x \in 0, 1, \dots, 52$) of the year. The parameter p has an important interpretation, as it is defined as the date of the POS, i.e., where the maximal NDVI value is reached.

The best fit for the curve parameters is found using the Trust Region Reflective algorithm (Conn et al., 2000). This generally robust optimization method finds the optimal set of parameters by minimizing the mean squared error (MSE) between the predicted NDVI curve and the NDVI data points. After the curve parameters have been fitted, we extracted the start SOS, POS and PEAK for each plot in each year.

The SOS is considered to be the time of year when the NDVI increases the fastest, i.e., the curvature of the NDVI curve increases the most. This can be calculated using the second derivative of the fitted curves. As shown in Fig. 3, the estimated start of season is the moment in time when the second derivative of the first logistic function is maximal. Combined with the aforementioned definition of the POS, we establish the following equation for calculating the relevant vegetation phenology characteristics:

$$\widehat{SOS} = \operatorname{argmax}_x - \frac{cb_1^2 e^{b_1(x-a_1)} (-e^{b_1(x-a_1)} + 1)}{(1 + e^{b_1(x-a_1)})^3} \quad (2)$$

¹ Data courtesy of the Icelandic Meteorological Institute.

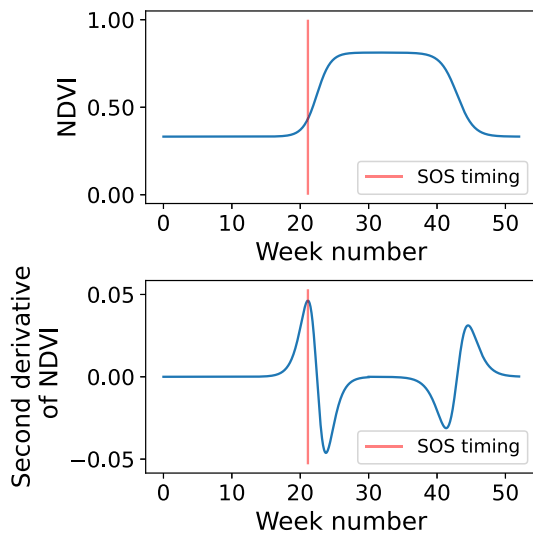


Fig. 3. The SOS is estimated based on the second derivative of the fitted NDVI curve. The SOS is defined as the week when the NDVI curvature increases the most, and is indicated with a red line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$$\widehat{POS} = p \quad (3)$$

$$\widehat{PEAK} = \widehat{NDVI}(p) \quad (4)$$

where \widehat{SOS} indicates the estimated start of the season, \widehat{POS} the date of the peak of the season, and \widehat{PEAK} the maximum value of the NDVI.

2.3. Statistical modeling and machine learning

2.3.1. Linear regression

After identifying the start and peak of the season for each plot and year, we performed a linear regression analysis. In this analysis, we used the SOS, POS, and PEAK as dependent variables, with the average soil temperature in each plot a year as the independent variable. We conducted this analysis using the ordinary least squares method available in the statsmodels library (version 0.13.2) for Python 3.9.13 (Seabold and Perktold, 2010). This approach also enabled us to compute the p -values for the slope and intercept of the linear model through a t -test. These p -values help us determine the statistical significance of the relationship between soil temperature and vegetation phenology characteristics by indicating whether the observed relationships are likely due to chance or reflect a genuine underlying pattern.

2.3.2. Machine learning

To better understand the inter-annual variability in our results, we used ML techniques to create models predicting different vegetation phenology characteristics. Specifically, we trained three separate MLPs: one to predict the start of the season, another to predict the peak of the season, and a third to predict the height of the peak season. An MLP is a type of ANN designed to mimic the way the human brain processes information. It consists of multiple layers of nodes (neurons): an input layer, one or more hidden layers, and an output layer which is used to provide the final predictions. Each node in a layer connects to every node in the next layer, with each connection having a specific weight. During training, the MLP adjusts these weights to minimize the difference between its predictions and the actual outcomes using an algorithm called backpropagation, allowing it to learn complex patterns in the data (Werbos, 1990).

Contrary to the linear models introduced in Section 2.3.1, the MLPs

also take meteorological variables into account. This meant that in total, each MLP used 79 input variables, which included the average weekly air temperature, precipitation and solar irradiance for the first 26 weeks of the year, as well as the average soil temperature over the entire year. We implemented the MLPs using the MLPRegressor class from the scikit-learn package (version 1.1.3) (Pedregosa et al., 2011). To ensure the models were as accurate as possible, we optimized their hyperparameters – the parameters that control the learning process – through a process called grid search, which we performed using Optuna (version 3.1.0) (Akiba et al., 2019). This process involved testing different combinations of hyperparameters to find the best settings for each of the three target variables. A description of these hyperparameters, the ranges we explored, and the optimal values we found are provided in Table 2.

To evaluate how well the models performed, we used three standard metrics: MSE, mean average error (MAE), and the coefficient of determination (r^2). For the grid search, we focused on minimizing the MSE to identify the optimal set of hyperparameters. Prior to conducting the grid search, we divided our data into a training set (80% of the data) and a test set (20% of the data). This split ensures that the models are trained on one portion of the data and tested on a separate, previously unseen portion, allowing us to assess their ability to generalize to new, unseen data accurately.

2.3.3. SHAP values

The 79 input features we used are not equally important, and each one influences the model's predictions differently. To understand which features are most significant, and what the direction of their impact is, we use SHAP values. They are calculated by examining how the model's predictions change when a specific feature is included or excluded, considering all possible combinations of features (Lundberg et al., 2017). By averaging these effects, SHAP values provide a clear and fair measure of each feature's contribution to the final prediction. This method ensures that the importance of each feature is assessed in the context of all other features in the model. In the end, SHAP values can break down each prediction made by the model, showing the contribution of each feature. The sum of the SHAP values for all features then equals the model's output.

After training the MLP models, we computed SHAP values using the model-agnostic Kernel SHAP method to understand which features are most important in predicting the start and (height of the) peak of the greening season. We used the implementation in the Python SHAP package for this analysis (Lundberg et al. (2017)).

Table 2

Overview of the explored ranges of hyperparameters used in the Optuna grid search. The optimal values for the three different regression tasks are displayed in the right-most three columns.

Description	Range	SOS	POS	PEAK
Number of neurons in first layer	int: 10, 20, ..., 100	100	70	30
Number of neurons in second layer	int: 0, 10, ..., 100	0	0	100
Strength of the L2 regularization term	float: 1e-4 — 1e-1 logscale	0.0290	0.0010	0.0606
the solver for weight optimization	adam, lbfgs	adam	adam	adam
initial learning rate	float: 1e-4 — 1e-1 logscale	0.0031	0.0003	0.0028
learning rate schedule for weight updates	constant, adaptive	constant	adaptive	adaptive
maximum number of iterations	int: 1000, 2000, ..., 10,000	8000	8000	8000
maximum number of iterations with no improvement	int, 10, 20, ..., 100	20	50	100

3. Results

3.1. The logistic fitting

For most plots and years, good fits were found for the double logistic curves that were fitted to the intra-annual individual plot NDVI data, with an average r^2 of 0.942 (± 0.095). However, for 5.8% of all plots and years, the data did not follow a double sigmoid curve, and the r^2 value was lower than 0.80. These curves were not included in the analysis. The mean estimated SOS was week 20.41 (± 2.40), the mean estimated POS was week 29.97 (± 3.27), and the mean estimated PEAK was 0.842 (± 0.071) across all the soil warming treatments.

3.2. The average response to soil temperature

Fig. 4 shows the linear relationship found between the average annual soil temperature and the three NDVI characteristics found by the double-logistic curves. The parameters of the linear model are given in Table 3. A significant linear relationship was found between average soil temperature and SOS ($p < 0.001$), POS ($p = 0.001$) and PEAK NDVI ($p < 0.001$) (Fig. 4 and Table 3). The relationship between soil temperature and SOS was negative, with an estimated coefficient of -0.2160 (± 0.053). This means that for every 4.63 degrees of soil warming, the greening season starts a week earlier. Otherwise stated, the SOS happens 1.52 days earlier per degree of soil warming when

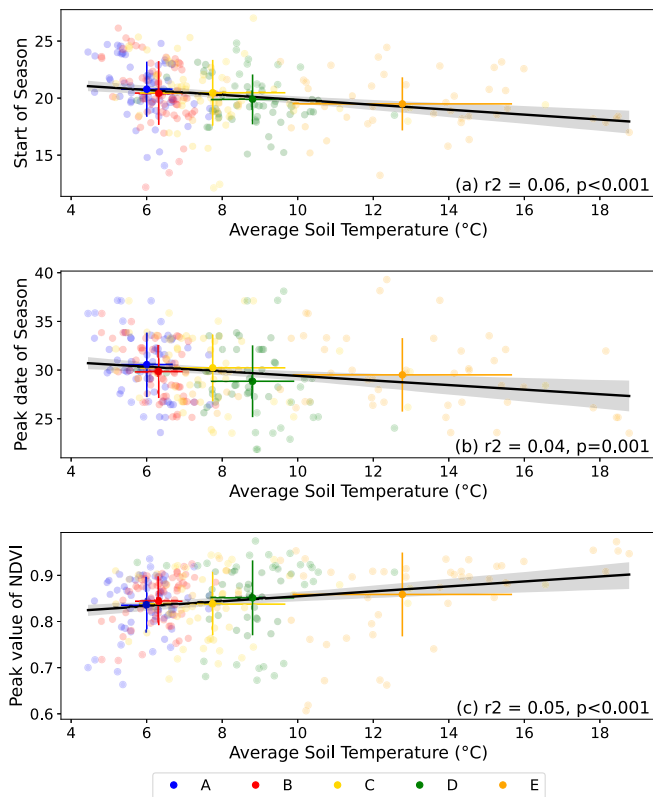


Fig. 4. Linear model that predicts the start of the season (a), the peak date of the season (b) and the peak value of NDVI (c), based on the average annual soil temperature. The filled circles represent the mean values for each category (A to E) of average soil temperature, with error bars indicating the standard deviation. The semi-transparent circles represent individual observations. The colour indicates the soil warming category where the blue points are A plots, the red points are B plots, the yellow points are C plots, the green points are D plots, and the orange points are E plots. All models had a significant relationship between the average soil temperature and the studied NDVI curve parameter (See Table 3). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 3

The parameters describing the results of the linear models, where different variables are fitted against the average soil temperature over a whole year. The SOS and POS are measured in weeks, while the intercept is measured in degrees Celsius.

Target variable	Slope	Intercept	r^2	p-value
SOS	-0.216 ± 0.052	22.011 ± 0.454	0.06	<0.001
POS	-0.235 ± 0.070	31.755 ± 0.607	0.04	0.001
PEAK	0.005 ± 0.001	0.801 ± 0.013	0.05	<0.001

derived across multiple years. Similarly, we see that the date of the NDVI peak shifted forward. The estimated coefficient of -0.2353 (± 0.07) indicates that for every 4.25 degrees of soil warming, the NDVI peaks a week earlier, or the POS occurs 1.65 days earlier per degree of soil warming. Finally, the PEAK value of the NDVI curve increased slightly with increasing soil temperature.

Although the linear relationships that were observed between average soil temperature and SOS, POS, and PEAK were significant (Fig. 4), we also observed a lot of unexplained variance, which is indicated by the relatively low r^2 values in Table 3.

3.3. The machine learning approach

To explain a larger part of the variance, the possibility of predicting characteristics of the NDVI curve using MLPs, based on both the soil temperature and meteorological variables, was investigated. The performance of the MLPs can be found in Table 4. From Tables 3 and 4, it becomes evident that the inclusion of the meteorological variables and the utilization of MLPs enabled us to explain a significantly larger part of the variance compared to the linear models.

To investigate the impact of a given feature on the predictions made by the model, we calculated SHAP values for all three MLPs. These can be found in Fig. 5, Fig. 6 and Fig. 7 for the SOS, POS and PEAK, respectively. In these figures, we separate the six years to investigate the annual variation in the SHAP values. To obtain the SHAP value for one meteorological variable, we summed the SHAP values of the 26 weekly averages, as shown in Eq. (5). Next, we calculated the sum of absolute values of the SHAP values A_SHAP for the four remaining features for all n samples, as shown in Eq. (6). By taking the absolute value and adding it over all years, we can investigate the total impact of a feature on the prediction, regardless of the direction of the impact. The results for the (A_SHAP) values are shown in Fig. 8.

$$\text{SHAP}_{\text{feature}} = \sum_{\text{week}=1}^{26} \text{SHAP}_{\text{feature,week}} \quad (5)$$

$$\text{A_SHAP}_{\text{feature}} = \sum_i^n |\text{SHAP}_{\text{feature},i}| \quad (6)$$

When interpreting Figs. 5 and 8a, we see that the meteorological variables had the largest impact on the prediction of the SOS. However, within each year, this impact was approximately constant. The intra-annual variation in the SOS was clearly the result of soil warming. In fact, the Pearson correlation between soil temperature and its accompanying SHAP values was -0.93 , meaning that the higher the soil

Table 4

Model performance of MLP after a 5-fold cross validation (CV) grid search. The test set consists of 20% of the total data, and is split evenly across the years of data taking. The naive MSE (MAE) is the MSE (MAE) when the mean of all training samples is used as the prediction.

Target	5-fold CV MSE	Test MSE (naive)	Test MAE (naive)	Test r^2
SOS	3.408	4.760 (7.102)	1.521 (2.095)	0.322
POS	7.933	8.943 (11.103)	2.473 (2.696)	0.192
PEAK	0.004	0.004 (0.006)	0.053 (0.063)	0.248

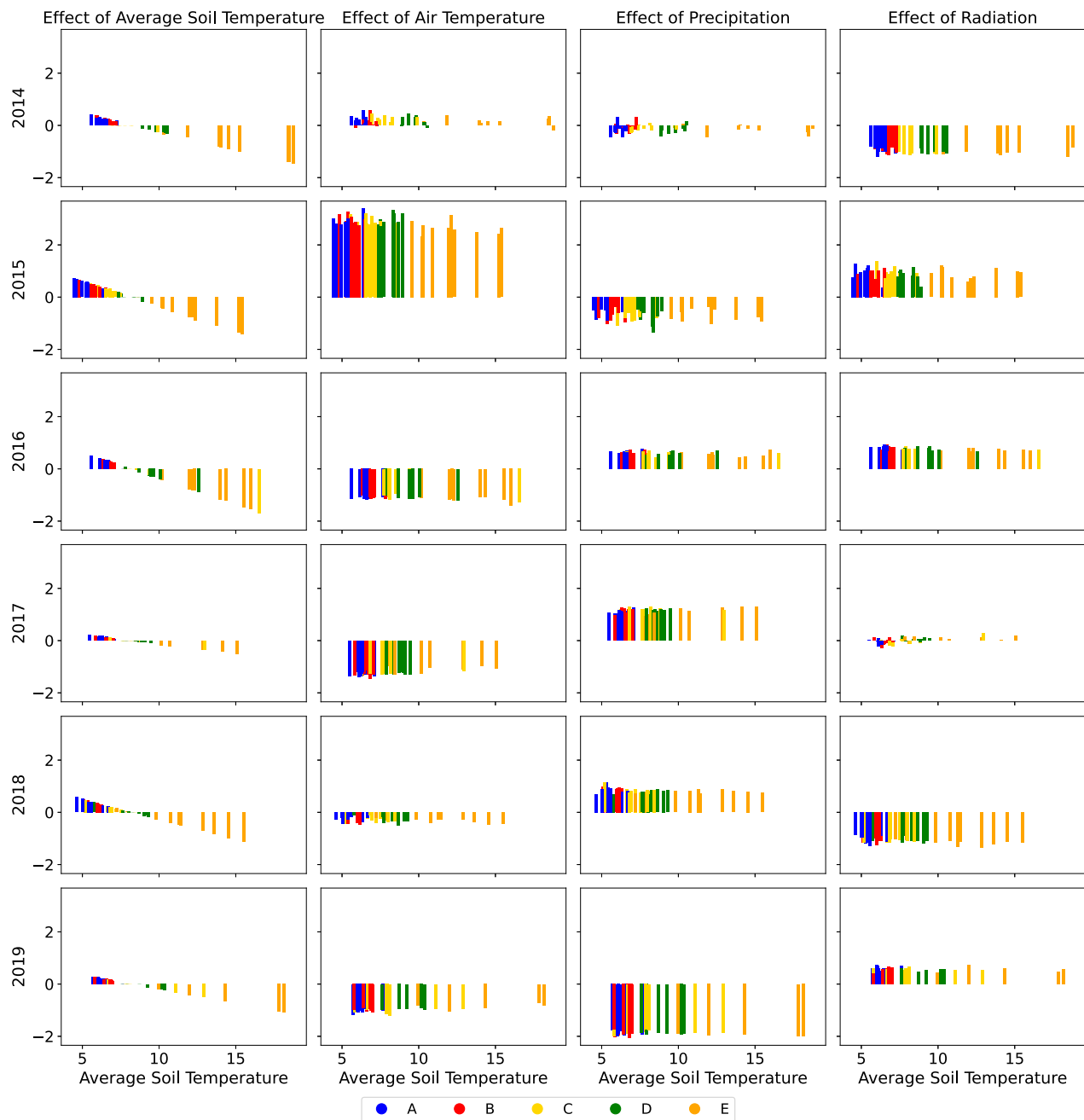


Fig. 5. SHAP values of multi-layer perceptron that predicts the start of the greening season based on the average soil temperature, air temperature, precipitation, and radiation. The colour indicates the soil warming category where the blue bars are A plots, the red bars are B plots, the yellow bars are C plots, the green bars are D plots, and the orange bars are E plots. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

warming, the earlier the season started each year. All Pearson correlation values can be found in [Table 5](#).

From [Fig. 8b](#) and [c](#), we can also conclude that the three meteorological variables also had the largest impact on the predictions of the POS and PEAK. From [Table 5](#), we can see that the POS was earlier and the PEAK value of the NDVI was higher with increasing soil temperature, as they had a Pearson correlation coefficient of -0.85 and 0.91 , respectively. For the POS, [Fig. 6](#) indicates that the size and direction of the SHAP effect for the three meteorological variables shifts significantly over the years, while the smaller effect of the soil temperature is relatively stable across the six years and drives the intra-annual variation within the dataset.

4. Discussion

The purpose of this study was to explore the relationship between soil temperature and NDVI, along with the impact of meteorological variables, utilizing ML techniques. The discussion will focus on emphasizing the novelties of this work, addressing the hypotheses presented in the paper, discussing the findings in relation to previous research, and highlighting the implications of the results.

4.1. Using machine learning to study vegetation phenology

Currently, the standard practice in vegetation phenology studies using NDVI consists of using traditional statistical methods such as (non-)linear regression or linear mixed models ([Estrella et al., 2021](#); [Hope](#)

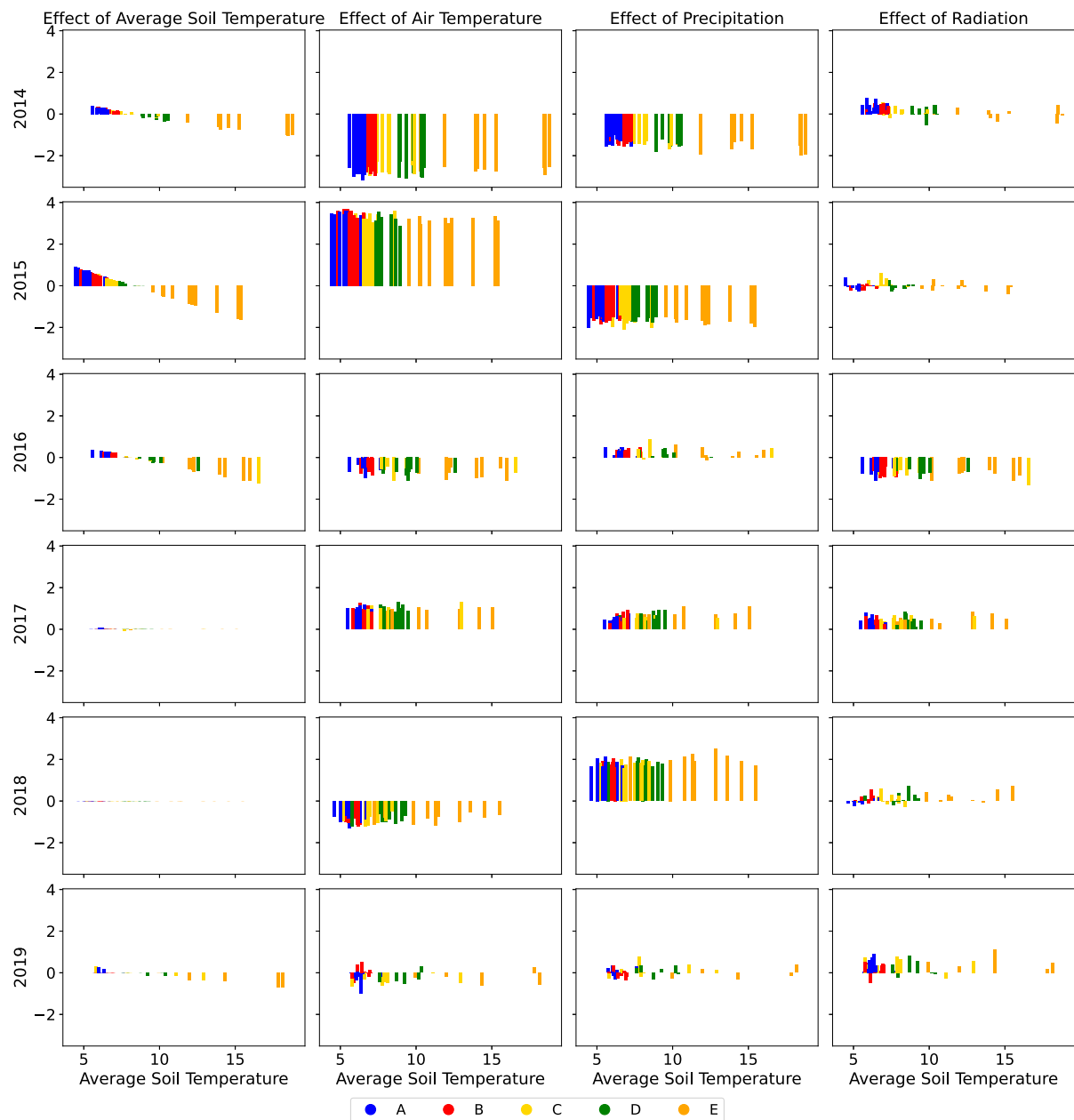


Fig. 6. SHAP values of multi-layer perceptron that predicts the peak of the greening season (POS) based on the average soil temperature, air temperature, precipitation, and radiation. The colour indicates the soil warming category where the blue bars are A plots, the red bars are B plots, the yellow bars are C plots, the green bars are D plots, and the orange bars are E plots. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

et al., 1993; Leblans et al., 2017; Mehmood et al., 2024; Walker et al., 2012a; Wang et al., 2021). However, our results clearly indicate that, after applying linear regression, a large amount of unexplained variance remains. Our study advances the traditional approach by using ML models, specifically MLPs, which integrate meteorological variables to capture nonlinear relationships. This method allowed us to explain a larger portion of inter-annual variance compared to traditional methods. The use of SHAP values further provided insights into a deeper understanding of the complex interactions between soil temperature, meteorological variables, and NDVI dynamics.

4.2. Effect of the soil temperature on SOS, POS, and PEAK in subarctic grasslands

The first hypothesis stated that a higher soil temperature would lead to an earlier SOS based on previous research by Leblans et al. (2017). Such responses have also been found when past changes in NDVI have been related to changes in annual, seasonal or monthly temperatures (Arndt et al., 2019; Karlsen et al., 2014; Potter and Alexander, 2020).

The findings of this study supported this hypothesis, as a significant relationship was observed between average soil temperature and the start of the greening season. The negative coefficient (-0.2160) indicates that SOS occurs 1.5 days earlier per degree of soil warming across the six years. This finding was consistent with a recent analysis from the International Tundra Experiment covering up to 20 years of

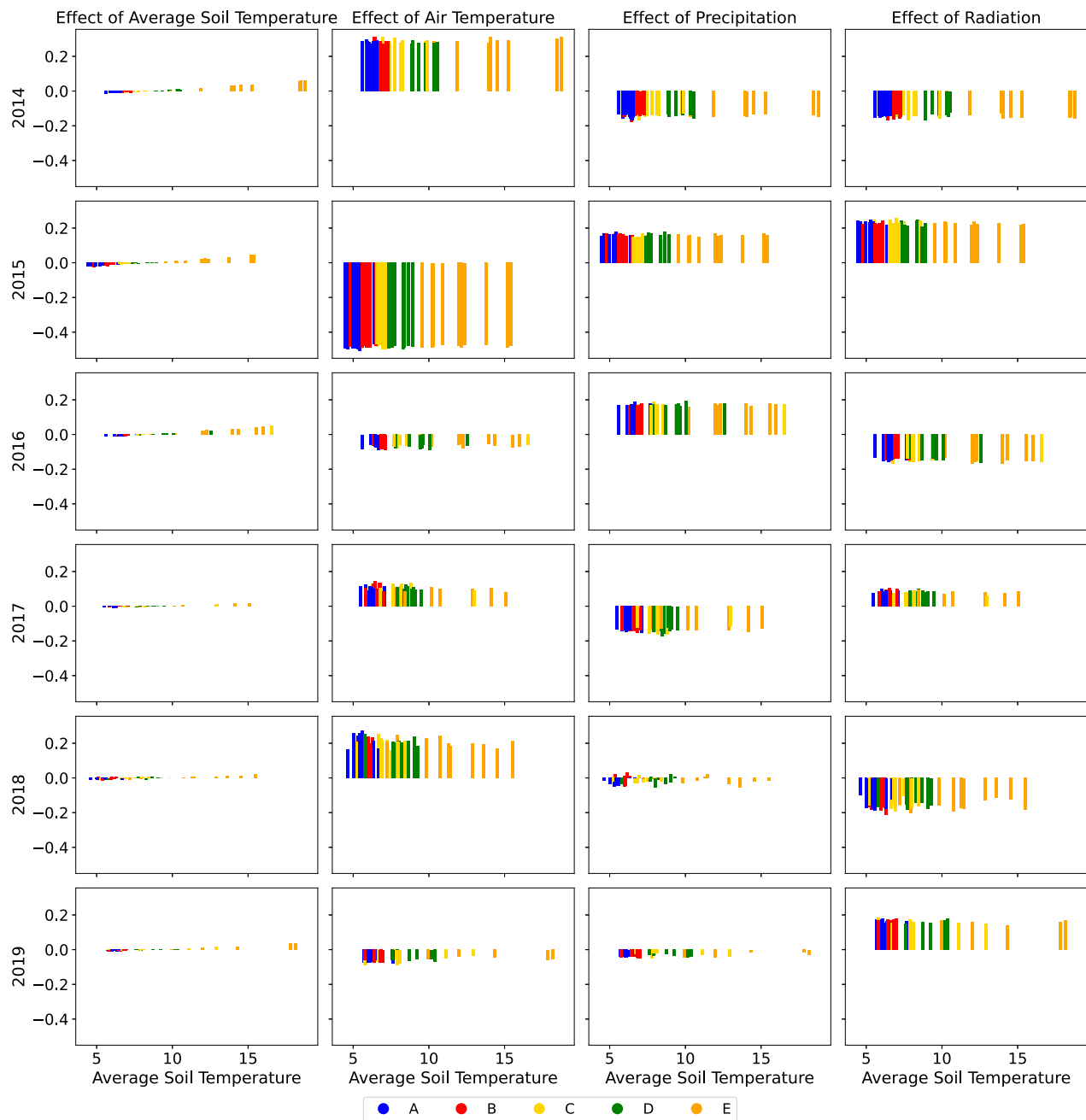


Fig. 7. SHAP values of multi-layer perceptron that predicts the peak NDVI based on the average soil temperature, air temperature, precipitation, and radiation. The colour indicates the soil warming category where the blue bars are A plots, the red bars are B plots, the yellow bars are C plots, the green bars are D plots, and the orange bars are E plots. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

data from 18 sites and 46 open-top chamber warming experiments across the Arctic, sub-Arctic, and alpine ecosystems (Collins et al., 2021). They observed a 0.73-day earlier start of the greening season, in an environment where the average air warming was 1.4 °C and the soil warming approximately half of that (Collins et al., 2021). Our finding was also consistent with previous research at the same ForHot site, as Leblans et al. (2017) found that on average, the SOS occurred 1.6 days earlier for every degree of soil warming.

Day length has traditionally been considered a dominant factor in regulating the phenology of many plant species (Adams and Langton, 2005; Roeber et al., 2022), particularly in high-latitude ecosystems where day length changes significantly throughout the growing season. Therefore in this study, the second hypothesis stated that the date of the POS would occur at a similar time each year, regardless of soil

temperature, as the day length remains consistent across all years. However, our results indicate that temperature conditions in the soil can have a considerable influence on the timing of POS. The hypothesis was therefore rejected. This finding suggests that, in our sub-Arctic grasslands, day length might not be the primary factor influencing the timing of the POS. While previous studies have highlighted the interplay between day length and air temperature in determining phenological events (Malyshev et al., 2014), our study is unique in demonstrating the notable impact of soil temperature. This underscores the need to consider soil temperature as an influential factor in phenological studies, particularly in the context of climate change where both soil and air temperatures are rising.

The third hypothesis proposed that the PEAK NDVI would not be significantly related to soil temperature, based on previous research by

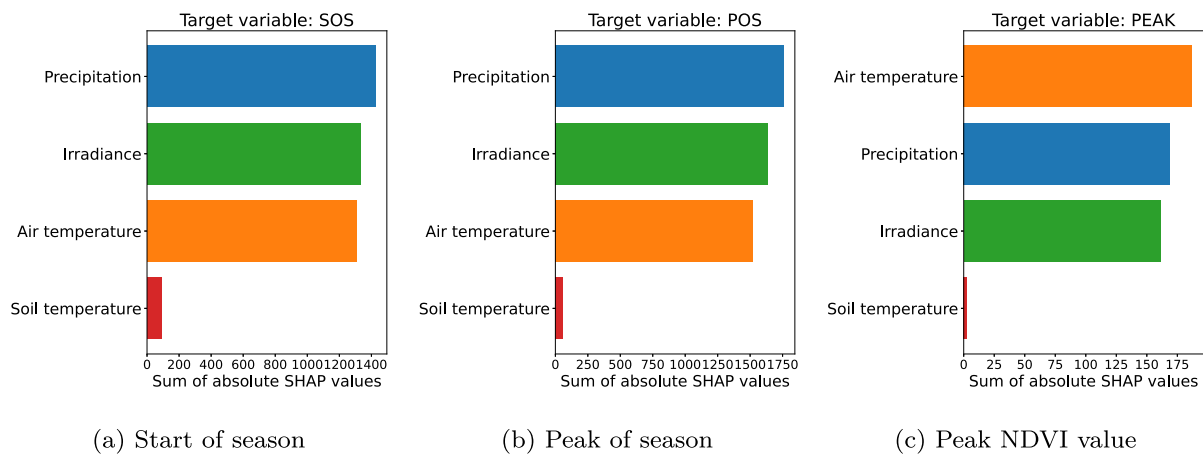


Fig. 8. Sum of the absolute SHAP values as defined in Eq. (6).

Table 5

Pearson correlation coefficient between the average soil temperature and its corresponding SHAP values.

Target variable	Pearson correlation
SOS	−0.93
POS	−0.85
PEAK	0.91

Verbrigghe et al. (2022a), who had not found significant differences in vegetation biomass across the warming gradients. However, the findings of this study indicate a slight increase in the PEAK value with increasing soil temperature. Although the relationship was not as strong as for the SOS and POS, it suggests that higher soil temperatures may contribute to higher NDVI peak values. It is worth noting that while NDVI is often used to estimate vegetation biomass (Bui et al., 2024; Lumbierres et al., 2017; Perry et al., 2022; Zhang et al., 2016), it is not measuring it directly, but rather the amount of chlorophyll per surface area (Huang et al., 2021). Therefore, “Arctic greening” measured using the NDVI, could occur without any changes in vegetation biomass, if the plants are getting “greener” due to a higher nutrient content in warmer soils. Further research is needed to better understand this relationship and its underlying mechanisms.

4.3. Effect of the other meteorological variables

Hypothesis B focused on the impact of other meteorological variables (air temperature, precipitation, and irradiance) on the inter-annual variability of the NDVI phenology and PEAK values, and the potential of ML to identify their importance. The results of the ML analysis using MLPs showed that these variables have a strong impact on the predictions of the SOS, POS, and PEAK, and the r^2 values of the MLPs were much higher than those obtained by the linear regression.

The SHAP values also provided information on the relative importance of these variables. It was noteworthy that the three meteorological variables had a much larger impact on the predictions than the soil warming data. These findings align with other studies that emphasize the significance of climatic variables over soil conditions because of their influence on soil temperature in predicting vegetation responses (Beer et al., 2018; Tan et al., 2022). However, the intra-annual variation in the SOS, POS, and PEAK was found to be influenced by the soil temperature. This influence of soil temperature highlights the significant role of below-ground processes in driving vegetation phenology and productivity (Fang et al., 2023). Studies have shown that soil temperature can affect root growth, nutrient availability, and microbial activity, all of which are crucial for plant development (Bhattarai et al.,

2023; Metz et al., 2024; Verbrigghe et al., 2022a). Understanding these interactions is essential for accurately predicting how the ecosystems will respond to ongoing climate change.

The SHAP values did not indicate significant differences among the meteorological parameters, making it challenging to prioritize their impact as hypothesized. This contradicts our hypothesis that air temperature's influence would be minimal due to its regulation of soil temperature, precipitation would have an intermediate effect, and irradiance would have a substantial impact, especially in cloudy sub-Arctic climates (Hou et al., 2015; Sigurdsson et al., 2016). However, collectively, these meteorological factors exhibited a considerably higher influence on the predictions compared to the soil warming data. Therefore, our findings not only contribute to understanding the dominant impact of meteorological parameters on vegetation dynamics, but also emphasize the need for continued research to explain the interdependencies and potential interactions between these factors.

4.4. Methodological considerations

It is important to note some limitations of the study. The analysis focused on a specific location in Iceland, and the results may not be directly applicable to other regions. The study period also covered a limited period of time (2014–2019), and longer-term data would provide a more comprehensive understanding of the inter-annual variation in NDVI. Furthermore, the meteorological data does not have the same spatial resolution as the NDVI or soil temperature data. Indeed, as we relied on the measurements of the nearest weather station, we had to assume that the weather conditions were the same across all plots.

The SHAP values should also be interpreted with caution. Although they are model-agnostic, we can only draw valid conclusions if the model generalizes well. That is, if it has an acceptable test set performance (Molnar et al., 2020). Furthermore, the SHAP values do not have a causal interpretation (Frye et al., 2020). We cannot assume that if the variable X has a large impact on the prediction of Y, then X causes Y. On the contrary, Y might cause X, X and Y could both be caused by a confounding variable, or they could have no causal relationship at all.

Nevertheless, this study produces valuable insights and provides clear directions for future research. Our promising results, achieved by applying ML in a vegetation phenology study, emphasize the potential of this approach in advancing our understanding of seasonal plant characteristics based on NDVI data. They can also be viewed as a starting point for other analyses in a broader ecological context.

In the future, it would be interesting to consider other model architectures or methodologies, for example, XGBoost (Chen and Guestrin, 2016). Additionally, other xAI approaches like LIME (Ribeiro et al., 2016) could be considered, allowing comparison between different xAI

approaches.

5. Conclusions

Our results only partly supported our hypotheses regarding the effect of soil temperature on the timing of the SOS, timing of the POS, and peak NDVI values. We observed a significant relationship between soil warming and the timing of SOS and POS, indicating that higher soil temperatures advance the onset of the growing season. Unexpectedly, this also led to a corresponding shift in the timing of POS. Moreover, the peak NDVI values showed a slight increase with higher soil temperatures. Furthermore, we explored the impact of meteorological variables, more specifically air temperature, precipitation, and irradiance, on vegetation phenology and its inter-annual variation. The use of SHAP values allowed us to gain insight into the relative importance and contribution of each meteorological variable to the predictions. It became evident that the three meteorological variables had the largest impact on the prediction of SOS, POS, and PEAK NDVI values across the six years. However, within a given year, the impact of the three meteorological variables remained approximately equal, while the variations in phenological characteristics were primarily driven by soil temperature.

For future work, we suggest further exploration of the underlying mechanisms driving the observed relationships between soil temperature and phenology. Investigating the physiological responses of plant species to soil temperature variations and exploring the interactions between soil temperature and other environmental factors at finer temporal and spatial scales would provide a more comprehensive understanding. Additionally, collecting data considering the soil characteristics, e.g., soil chemistry or nutrient availability, could improve the performance of the ML models, and further increase the explained variance.

In addition, incorporating advanced remote sensing techniques, such as satellite imagery, in conjunction with ground-based measurements can improve the accuracy and comprehensiveness of phenological studies in subarctic grassland ecosystems. Long-term monitoring at multiple sites and the incorporation of various geographical locations would provide valuable information on the generalizability of our findings and the response of subarctic grasslands to ongoing climate change.

This study contributes to our knowledge of the relationships between soil temperature, other meteorological variables, and vegetation phenology in subarctic grassland ecosystems. The findings enhance our understanding of the mechanisms driving ecosystem dynamics in these regions and have implications for predicting and managing subarctic grasslands in the face of environmental change. Finally, this work also functions as a proof-of-concept for ML-based vegetation phenology studies, and thereby provides a solid foundation for future research in this domain.

CRedit authorship contribution statement

Steven Mortier: Conceptualization, Methodology, Software, Validation, Formal analysis, Data Curation, Writing - Original Draft, Visualization, Writing - Review & Editing. **Amir Hamedpour:** Conceptualization, Methodology, Investigation, Writing - Original Draft, Visualization, Writing - Review & Editing. **Bart Bussmann:** Conceptualization, Methodology, Software, Data Curation. **Ruth Phoebe Tchana Wandji:** Conceptualization, Methodology, Investigation, Writing - Original Draft, Writing - Review & Editing. **Steven Latré:** Funding acquisition, Supervision. **Bjarni D. Sigurdsson:** Investigation, Writing - Review & Editing, Funding acquisition, Supervision, Project administration. **Tom De Schepper:** Conceptualization, Methodology, Writing - Review & Editing, Supervision. **Tim Verdonck:** Conceptualization, Methodology, Resources, Writing - Review & Editing, Supervision.

Data availability

The data used in this study is made available as open data and can be found here: <http://dx.doi.org/10.17632/C9T7FX9N4H.1> (Mortier et al., 2023).

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