Estimating pasture quality of Mediterranean grasslands using hyperspectral narrow bands from field spectroscopy by Random Forest and PLS regressions

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Abstract

Mediterranean grasslands are a cornerstone ecosystem to provide ecosystem services and sustain human societies. The sustainability and provision of ecosystem services by these systems rely on their management. One of the main attributes to perform sustainable and effective management is pasture quality, which is crucial for animal performance in rainfed extensive systems. Remote sensing of grasslands can be an effective tool to inform the management of grasslands. The forthcoming high-priority mission candidate of the European Space Agency, Copernicus Hyperspectral Imaging Mission for the Environment (CHIME) with continuous narrow bands of ≥10 nm spectral resolution could be an asset to provide accurate information on the pasture quality of high-diverse and heterogeneous grasslands. In this study, we investigated the potential of CHIME-like field spectroscopy data at 10 nm resolution to assess the quality of Mediterranean permanent grasslands. The pasture quality indicators used were: crude protein (CP), neutral detergent fibre (NDF), acid detergent fibre (ADF) and enzyme digestibility of organic matter (EDOM). To do so, two machine learning methods commonly used in remote sensing were implemented: Partial Least Squares (PLS) regression and Random Forest (RF) regression. The results using all bands in the 400-2300 nm spectral range and the results obtained by Backward Feature Elimination

(BFE) were also compared. Finally, using importance measures of PLS and RF and the BFE approach, the importance and stability of the bands to assess the pasture quality indicators were explored. The results showed that field spectroscopy CHIME-like data at 10 nm of spectral resolution show potential to predict CP at “good” accuracy and NDF at “moderate” accuracy level in Mediterranean permanent grasslands. PLS outperformed RF to predict CP and NDF in terms of accuracy and certainty of the predictions. The BFE approach increased the accuracy of the predictions, especially in PLS, for which a ΔRMSE= -12.5 was achieved in cross-validation to predict CP. The models built by BFE approach to predict CP using PLS provided a mean R^2 value of 0.82 and a range of 0.68-0.90 in bootstrapped predictions. The RMSE was low (mean RMSE=2.23%) and the mean RPD=2.47 with values ranging from 1.81 to 3.23. RF models to predict CP produced mean R^2 value of 0.68, mean RMSE=3.00% and mean RPD=1.82. ADF and EDOM were predicted with poor accuracy and similarly by both, PLS and RF. The bands located in the red-edge and NIR region showed high importance and stability to assess the best-predicted variables. Bands centred at 700, 710, 1160, 1170 and 1180 are highly stable and important to predict CP. The bands from the SWIR region had lower stability. This study provides insightful results on the use of hyperspectral data and future satellite missions such as CHIME to assess the pasture quality of Mediterranean grasslands that can be crucial to inform the management and monitoring of Mediterranean permanent grasslands.

Keywords: Crude protein, Band selection, Backward feature elimination, CHIME, Band importance, Heterogeneity

1. Introduction

The high diversity of vascular plants, strongly related to the management practices and characteristics of the Mediterranean climate, make the Mediterranean Basin a global biodiversity hotspot (Cosentino et al., 2014; Myers et al., 2000). Grasslands of the Mediterranean-climate zones contribute substantially to the biodiversity of the Mediterranean Basin and have traditionally played a major role to sustain human livelihood (Jouven et al., 2010; Porqueddu et al., 2016). Mediterranean grasslands are mainly annual high-diverse communities of grasses, legumes and forbs, of low biomass production due to the low rainfall and its high intra- and inter-annual variability which together with the grazing and occasional cropping are responsible for the strong heterogeneity of this ecosystem (Cosentino et al., 2014; Olea and San Miguel-Ayanz, 2006; Porqueddu et al., 2016). In the last decades, increasing attention has been directed to the potential of Mediterranean grasslands ecosystems to provide multiple ecosystem services highly appreciated by the society and of crucial importance for the global environment such as biodiversity conservation, wildfires control and rural population sustain (D'Ottavio et al., 2018; Porqueddu et al., 2016; Porqueddu et al., 2017).

Mediterranean grasslands are associated with extensive livestock grazing by small ruminants and beef cattle (Cosentino et al., 2014) that act as a major driver determining stability, sustainability, and potential of ecosystem services provision (D'Ottavio et al., 2018; Porqueddu et al., 2017; Sollenberger et al., 2019). The increasing effects of climate change challenge the stability and functions of Mediterranean grasslands compromising their resilience (Giannakopoulos et al., 2009; Giorgi and Lionello, 2008; Chang et al., 2017; Ma et al., 2017, Carpintero et~~l~~ al., 2020). In this context, it is crucial to have accurate and routine information on the attributes of grasslands to i) improve the economic, environmental sustainability and efficiency of grassland management at farm level, and ii) monitor their dynamics and conservation status at a larger scale. One of the most important attributes of grasslands concerning their management for livestock rearing is the pasture quality. Pasture's quality can be understood in many ways, but in the context of animal feeding, it usually refers to proximate nutritional principles (Dumont et al., 2015) such as crude protein and fibre, ether extract, minerals, ash, or the energy provided (Pullanagari et al., 2013).

The main methods to assess pasture quality are: i) laboratory-based methods, ii) proximal remote sensing, iii) aerial remote sensing (aircraft~~s~~ and UAVs) and iv) space-based remote sensing (Pullanagari et al., 2013). The accuracy of the estimations is reduced following the order in with these methods have been listed (Pullanagari et al., 2013). Laboratory-based methods are the standard and commonly used ~~methods~~ to assess pasture quality. However, through the previous calibration using reference data determined by laboratory methods, indirect methods based on the remote sensing of the pasture reflectance are gaining importance in pasture quality determination. Concerning the cost, laboratory-based methods are the most expensive methods due to laborious manual sampling collection and analysis compared to the sensing methods (Starks et al., 2004). Within the sensing methods, satellite technology is especially interesting because of the large-scale coverage and regular data provision. In particular, Sentinel-2 satellites have demonstrated a great potential to monitor grasslands ecosystems (Askari et al., 2019; Fernández-Habas et al., 2021; Raab et al., 2020; Ramoelo et al., 2014; Sibanda et al., 2015) due to the free provision of multispectral data at worldwide level with a frequency of 5 days (ESA, 2021). However, because of the intrinsic heterogeneity of Mediterranean grasslands, multispectral data might have limited potential to provide accurate information on quality grasslands attributes (Fernández-Habas et al., 2021). The European Space Agency has a new high-priority mission candidate Copernicus Hyperspectral Imaging Mission for the Environment (CHIME) (Nieke and Rast, 2018; Rast et al., 2019). The objective of this mission is: *“To provide routine hyperspectral observations through the Copernicus Programme in support of EU- and related policies* *for the management of natural resources, assets and benefits"*. According to the Mission Requirements Document, this imaging spectrometer will measure in the 400-2500 nm spectral range with continuous narrow bands of ≥10 nm spectral resolution, spatial resolution of 20-30 m and revisiting time of 10 to 12.5 days (Nieke and Rast, 2018; Rast et al., 2019).

In addition to satellite sensors, field spectroscopy has also demonstrated great potential and applicability to in-field pasture quality assessments (Pullanagari et al., 2012). Field spectroscopy has also been used to upscale models to satellite data and to simulate the applicability of different satellite spectral resolutions (Fernández-Habas et al., 2021; Lugassi et al., 2019; Mutanga et al., 2015; Ramoelo and Cho, 2018; Sibanda et al., 2015). In this study, we apply this approach to investigate the potential of the CHIME mission to assess the quality of high-diverse Mediterranean permanent grasslands.

Machine learning algorithms have a great potential to exploit hyperspectral data and to retrieve grasslands attributes (Verrelst et al., 2015). The number of variables is usually larger than the number of samples and, on the other hand, these data tend to suffer from multicollinearity (Adjorlolo et al., 2013; Rivera-Caicedo et al., 2017). The redundancy and correlation between variables in hyperspectral data lead to the 'Hughes phenomenon' where the accuracy of the classification/predictions increases gradually with an increasing number of spectral bands or dimensions to a certain number of bands when it decreases dramatically (Hughes, 1968; Ma et al., 2013). Therefore, the algorithms used have to be efficient in dealing with these issues to avoid the 'Hughes phenomenon', also known as 'curse of dimensionality' (Rivera-Caicedo et al., 2017; Verrelst et al., 2015).~~The algorithms used have to be efficient in dealing with these issues to avoid the Hughes phenomenon (Verrelst et al., 2015)~~. Two methods are commonly used in remote sensing and chemometrics to analyse hyperspectral data:

Partial Least Squares (PLS) regression and Random Forest (RF) regression. These methods have been extensively implemented in remote sensing demonstrating their robustness and reliability (Verrelst et al., 2015). PLS is the state-of-the-art non-parametric method for analysing spectroscopic data~~, widely used in chemometrics~~ (Kucheryavskiy, 2018; Wold et al., 2001) and vegetation properties mapping (Biewer, et al., 2009b; Verrelst et al., 2015). RF is an ensemble classification and regression algorithm consisting of an evolution Classification and Regression Trees (CARTs) developed by Breiman (2001) that combines bagging and bootstrapping approaches. It has become popular for remote sensing applications due to its high accuracy, flexibility to be used with complex datasets and few hyperparameters to be set (Belgiu and Drăgu, 2016).

Previous studies have provided insightful information about the potential of field spectroscopy at different spectral resolutions (Pullanagari et al., 2012). For example, Zhou et al. (2019) demonstrated the feasibility of the Yara N-sensor spectrometer at 10 nm spectral resolution to predict the yield and quality of legume and grass mixtures. The recently published research by Pullanagari et al. (2021) provided conclusive results about the prediction of canopy nitrogen concentration in temperate grasslands by a convolutional neural network, PLS and gaussian process regression using field spectroscopy.

Although PLS and RF can deal with multicollinearity, feature selection approaches are highly recommended when using hyperspectral data due to the issues mentioned above (Belgiu and Drăgu, 2016). Several studies have demonstrated that predictions using both PLS and RF can benefit from data reduction by feature selection in hyperspectral data (Mansour et al., 2012; Belgiu and Drăgu, 2016; Kawamura et al., 2008). Another important application of this approach is the identification of important bands or the removal of redundant information. PLS and RF can also provide estimates of the bands importance (Belgiu and Drăgu, 2016; Mehmood et al., 2012; Santos-Rufo et al., 2020). This information has relevant implications to: i) inform the use of hyperspectral data ii) optimise the models and data used and iii) inform the design of hyperspectral-based devices (Chan and Paelinckx, 2008; Pullanagari et al., 2012). These approaches of band selection and band importance identification have direct application to the use of the data provided by the forthcoming CHIME mission whose spectrometer is expected to be equipped with 210 bands (Nieke and Rast, 2018). In fact, the Mission Requirements Document by Rast et al. (2019) pointed out that one of the following analyses of the Mission would be to *"confirm the spectral sampling requirements (10 nm at FWHM) for the target applications and related products, incl. support to product quality specification"*. To the best of our knowledge, the applicability of hyperspectral narrow bands to assess the pasture quality of Mediterranean grasslands has received poor attention. Given the particularities (high heterogeneity and variability) and interest of these ecosystems outlined before, further research focused on this type of grasslands is required to advance in the use of sensing methods in their management and monitoring.

In this context, the overall objective of this study was to assess the potential of hyperspectral data CHIME-like at 10nm spectral resolution to estimate pasture quality in Mediterranean permanent grasslands using field spectroscopy. To achieve this goal, we established the following specific objectives:

i) Evaluate and compare the performance and prediction accuracy of RF and PLS regressions to assess crude protein (CP), neutral detergent fibre (NDF), acid detergent fibre (ADF) and enzyme digestibility of organic matter (EDOM).

~~ii)~~ Test the implementation of backward feature elimination techniques (BFE) to optimise the predictive models~~.~~ and to

~~iii)~~ii) ~~I~~identify the most important narrow bands to predict the pasture quality indicators.

~~iv)~~iii) Interpret the implications of the outcomes for the management and monitoring of Mediterranean permanent grasslands.

2. Material and methods

2.1. Pasture sampling

Pasture samples were taken in five *Dehesa* farms from the Cordoba province, in the north of Andalusia region (Spain) during the growing season of 2012-2013 (farms 1-4) and 2018-2019 (farm 5) (~~Table 1~~Fig. 1). The pasture sampling conducted in 2012-2013 was aimed at studying the grazing effect on pasture quality of natural permanent grasslands of *Dehesas* in a previous study (Fernández et al., 2014). Four sampling quadrats of 0.4 x 0.4 m were randomly set within grazing exclusion plots and four outside of them. This sampling was repeated on five dates; January/February, March, April, May and June which provided 125 samples (Table 1) after removal of those with extremely low pasture biomass for laboratory analysis. Locations of 0.4 x 0.4 m quadrats sampled on previous dates were avoided. In farm 5, pasture samples were collected in May of 2019. Plots of 10x10 m were located in irrigated grasslands (3 plots) natural grasslands (3 plots) and improved grasslands with commercial seed mixtures (6 plots). Within each 10 x 10 m plot, four sampling quadrats were randomly set, providing 48 pasture samples. The pasture contained within the quadrats was clipped to ground level, dried in the oven for 48 h at 60ºC and ground to pass through a 1-mm sieve. In total, 173 samples (Table 1) were analysed at the Laboratory of Animal Nutrition of SERIDA (Villaviciosa, Asturias, Spain) to determine the percentage of crude protein (CP), neutral detergent fibre (NDF), acid detergent fibre (ADF) and enzyme digestibility of organic matter (EDOM). The grasslands sampled consisted of communities mainly dominated by annuals with species such as *Avena* spp., *Astragalus pelecinus, Bromus* spp., *Diplotaxis* spp., *Erodium* spp., *Hordeum* spp., *Lolium* spp., *Ornithopus compressus, Plantago* spp., *Trifolium subterraneum*, *T. cherleri*, *T. tomentosum*, *T. glomeratum*, and *Vulpia* spp in natural grasslands, *T. repens* and *Lolium* spp., in the irrigated field and *T. vesiculosum*, *T. michelianum*, *T. resupinatum*, *O. compressus* and *L. multiflorum* in improved grasslands from farm 5.

2.2. Canopy reflectance measurement and preprocessing

Before pasture clipping, the reflectance of the pasture contained in the 0.4x0.4 m quadrats was recorded using an ASD FieldSpec Spectroradiometer (ASD Inc, Boulder, Colorado, USA). The measurements were taken under clear sky between 10:00 and 15:00. The spectroradiometer records reflectance at a spectral resolution of 1.4 nm within the 350-1000 nm range and 2 nm within the 1000-2500 nm range. The output data is an interpolated reflectance at 1 nm spectral resolution in the whole range of 350-2500 nm. The device is equipped with a fibre optic probe assembled to a pistol grip that is held at 1.20 m height resulting in a 0.22 m^2 measurement area. Four replicated were recorded per quadrat and averaged to provide a unique representative reflectance measurement of the quadrat. Calibrations on white references were done on a Spectralon panel (Labsphere, NorthSutton, NH) every four samples.

The spectra were smoothed applying the Savitzky-Golay (Savitzky and Golay, 1964) filter using a width of filter window of three and second-order of polynomial. Those regions of the spectra displaying noise due to instrumental noise (350-395 nm and 2300-2500 nm), atmospheric noise (1370-1410 nm and 1816-1941 nm) or detector change (1000-1005 nm) were removed. In order to match the spectral specifications of the high-priority candidate mission of the European Space Agency: Copernicus Hyperspectral Imaging Mission for the Environment (CHIME) (Nieke and Rast, 2018), the spectra were resampled to 10 nm spectral resolution using the *"resample2"* function of the CRAN-package "*prospectr*" (Stevens and Ramirez-Lopez, 2015) resulting in 168 hyperspectral bands of 10 nm resolution. Spectral outliers were identified by principal component analysis (PCA) (Morellos et al., 2016; Xu et al., 2018). All analyses, preprocessing and modelling were performed in R v. 3.6.1 (R Development Core Team, 2019).

2.3. Partial Least Squares

PLS consist of a lineal multivariate regression model that relates a *Y* matrix of response variables (CP, NDF, ADF or EDOM) with an *X* matrix of predictor variables (168 hyperspectral bands) by decomposing both *Y* and *X* in n-orthogonal Latent Variables (LV) to maximise their covariance. PLS models were calibrated by Leave-One-Out cross-validation (LOOcv). The only parameter to be adjusted in PLS, the optimal number of LV, was selected based on the first local minimum of the root mean squared error (RMSE) of the cross-validated predictions. In this study we describe the basic functioning and characteristics of PLS, further information can be found on Geladi and Kowalski (1986), De Jong (1993) and Wold et al. (2001). PLS models were implemented using CRAN-package *"mdatools"* (Kucheryavskiy 2019; Kucheryavskiy 2020).

2.4. Random Forest

The RF regression is a machine learning technique that uses the ensemble of a set of Classification and Regression Trees (CARTs) to make predictions (Breiman, 2001). By bagging approach, RF uses two-thirds of the samples (*in-bag* samples) to create *n* user-defined unpruned and independent trees (*ntrees*). The remaining third of the samples, the so-called *out-of-bag* (OOB) samples, are used to estimate the Mean Squared Error (MSE), known as the OOB error. The OOB error is considered an accurate estimate of the performance of the model (Grimm et al.,2008; Liaw and Wiener, 2002; Mutanga et al., 2012). At each node of the regression trees, instead of choosing the best split among the predictors as in CARTs, RF randomly selects a~~n~~ user-defined number of predictors (*mtry*) (Liaw and Wiener, 2002). The final predicted value is obtained by averaging the predictions of the *ntrees*. The RF algorithm was implemented with CRAN-package *"randomForest"* (Liaw and Wiener, 2002). As explained above, RF has two main~~s~~ hyperparameters, the number of trees to grow (*ntree*) and the number of predictors to select at each node (*mtry*). The default values of *"randomForest"* were used for *ntree* (500 trees) and *mtry* (1/3 of the total number of ~~predictros~~predictors) since they have shown to be acceptable values and the most common recommendation (Belgiu and Drăgu, 2016; Díaz-Uriarte and Alvarez de Andrés, 2006). To ensure the right choice of these parameters, RMSE was calculated with the default of *mtry*, half of the default, and twice the default as suggested by Liaw and Wiener (2002).

2.5. Band importance and selection by backward feature elimination in PLS and RF

The modelling approach followed in this study is schematised in ~~Fig. 1~~Fig. 2. Band importance in PLS models was measured based on the absolute value of the regression coefficients which is a *"single measure of association between each variable and the response"* (Mehmood et al., 2012). Bands with a large absolute magnitude of their associated regression coefficients are expected to have a high impact on the models while small absolute values of regression coefficients indicate that these bands are unimportant or redundant (Garrido Frenich et al., 1995; Kawamura et al., 2008). This technique has shown to be a robust method in variable selection with PLS (Garrido Frenich et al., 1995; Palermo et al., 2009).

The most reliable method for variable importance estimation in RF is the so-called "permutation importance". The rationale of this method consists of randomly permuting a predictor variable X_j (band in this case) and calculating the MSE of the prediction of the OOB set with the remaining predictors. The difference between the MSE when X_j is permuted and the baseline MSE calculated with all predictors (measured as the percentage increase of MSE) is a measure of the variable importance (Strobl et al., 2007). This process is repeated over all predictors. If the predictor X_j is strongly associated with the response, its exclusion from the predictors produces a substantial increase in the MSE.

The most important bands for the prediction of the studied pasture quality variables were selected based on backward feature elimination (BFE). The BFE in PLS was carried out by means of the filter method based on removing at each iteration the band with the smallest absolute value of its regression coefficient (Mehmood et al., 2012). After removing the least important band, a LOOcv is performed to select the optimal number of LV and the new regression coefficients recalculated. This process was repeated until only two bands were left. At each step, the coefficient of determination (R^2) and the RMSE of the LOOcv are calculated. A similar method was applied to RF. The least important band (based on the lowest increase in MSE) was removed at each step until only two bands were left (Adam et al., 2014; Díaz-Uriarte and Alvarez de Andrés, 2006; Odindi, 2014). The R^2 and the RMSE of the OOB estimation were also calculated at each step. The selection of the most important set of bands was determined by selecting the model that yielded the highest R^2 and the lowest RMSE of LOOcv and OOB estimates in PLS and RF respectively in the BFE process.

To study the effect of the dataset and the stability of the selected bands, the BFE process was repeated n=100 times over 70% of samples selected by bootstrap. The percentage of times that the bands were selected in the 100 repetitions of the BFE was used as an estimate of their stability.

2.6. Assessment of performance and predictive ability of PLS and RF models

Following Kawamura et al. (2008), Mutanga et al. (2004) and Mutanga et al. (2015) a bootstrap approach was applied to test the performance, robustness and predictive ability of the models built with the selected bands by BFE. The original dataset (n=164) was randomly split into 70% for calibration and 30% for independent test. This random split was repeated 100 times. For both, PLS and RF, models were built with the calibration set (70% bootstrapped samples) to predict over the remaining 30%. The R^2, RMSE and Ratio of Performance to Deviation (RPD) of the test predictions were recorded. Mean and confidence intervals (CI) (2.5 and 97.5 percentiles) of R^2, RMSE and RPD were calculated and reported. Following Askari et al. (2015), the performance and predictive ability of the models were assessed considering the thresholds: "poor" accuracy (RPD < 1.5 and $R^2 < 0.6$), "moderate" ($1.5 \leq$ RPD<2 and $R^2 \geq 0.60$), "good" ($2 \leq$ RPD< 2.5 and $R^2 \geq 0.7$) and "excellent" (RPD ≥ 2.5 and $R^2 \geq 0.8$).

3. Results

3.1. Statistics of pasture quality variables

Table 2 shows the descriptive statistics of CP, NDF, ADF and EDOM. There was a wide range of data and large variability for all variables. CP had the largest CV with 45.4 % while the rest of the variables had a CV close to 19%. These variables also showed high variability across the different dates of sampling (Fig. S1).

3.2. Performance of PLS and RF models with all bands and with bands selected by backward feature elimination

The PCA of the spectral data revealed nine points laying outside the 95% confidence ellipse (~~Fig. 2~~Fig. 3) that were omitted from the dataset used in the analysis.

Overall, the best models were obtained for CP, with R^2 values over 0.70 using all bands and the selected bands with both PLS and RF, having also the smallest RMSE values. R^2 values for NDF were in the range of 0.52-0.67 and between 0.47-0.59 for EDOM. ADF was the parameter that showed the worst statistics with R^2 always below 0.50. PLS outperformed RF in both cases, with all bands and with selected bands for all variables (Table 3). The backward feature elimination improved the performance of the models for all pasture quality variables and for both regression methods, PLS and RF. The ΔRMSE denotes that the improvement was different depending on the variable and always higher for PLS (Table 3). The greatest improvement (-12.5 ΔRMSE) with selected bands was obtained for CP with PLS regression, which was the model that showed the best performance with R^2=0.84 and RMSE=2.17 using 21 bands.

~~Fig. 3~~Fig. 4 illustrates the changes of R^2 and RMSE in backward feature elimination in PLS and RF regressions. In both R^2 and RMSE, the changes in PLS models are more evident than in RF, in which the changes are steadier. In the same line, in PLS both parameters R^2 and RMSE show abrupt changes just after the optimal number of bands selected (~~Fig. 3~~Fig. 4). However, in RF after this point, there is a steady interval until the values drop rapidly. RF showed the best results or negligible variations with the default value of mtry=1/3 and stabilisation of RMSE before the 500 trees are grown (~~Fig. S4~~Fig. S5 and ~~Fig. S5~~Fig. S6) (Belgiu and Drăgu, 2016; Díaz-Uriarte and Alvarez de Andrés, 2006; Liaw and Wiener, 2002).

3.3. Bands selected by backward feature elimination and importance in PLS and RF

The number and proportion of bands selected by backward feature elimination for each pasture quality variable are shown in Table 3. Several differences can be observed between models. PLS tended to select fewer bands than RF in all variables. The variable with a higher proportion of bands selected using backward feature elimination was NDF, for which 15.5% and 48.8% of the bands were selected with PLS and RF respectively (Table 3). Only 7 bands were selected for ADF with PLS while 53 bands were selected using RF. For CP and EDOM, 12.5% and 10.1% were selected with PLS and 32.7% and 20.2% using RF.

The position of these selected bands in the spectral range of 400-2300 nm is illustrated in ~~Fig. 4~~Fig. 5. This figure also illustrates the reflectance curve depending on the content of the pasture quality variable. It can be observed how samples with high values of CP and EDOM and low fibre content show higher reflectance values in the Near Infra-Red region (NIR) (800-1300 nm). Again, some differences can be observed between models. Especially concerning the visible region, while in RF the bands located in this region are mostly selected, in PLS these bands are almost absent. The same happened in the region between 800 nm and 900 nm, in which just band 880 was selected for NDF in PLS, whereas in RF several bands were selected in this spectral region.

Bands from the red-edge region (680-750 nm) were commonly selected for all variables using both PLS and RF (~~Fig. 4~~Fig. 5). Especially the band centered at 700 nm was selected for all models but ADF using PLS. This band also showed high importance and stability in the predictions (Fig. 6~~4.~~). For example, for the predictions of CP with PLS and RF, this band was the second and the most important band respectively, having also the highest value of stability (Fig. 6~~4.~~).

Bands from the NIR (800-1300 nm), especially from 900 nm onwards in PLS, and the shortwave infrared region (SWIR) from 1300-2300 were also intensively selected in most of the variables using both, PLS and RF except for ADF using PLS. Bands 960 and 1160 for example were selected with PLS in CP (Fig. 6~~4.~~), and NDF (~~Fig. S1~~Fig. S2.). Band 1960 was selected in all models for CP and NDF.

Fig. 6~~5~~ shows the importance of the bands selected with PLS and RF for CP prediction. The importance for the rest of the variables can be consulted on Supplementary Material (Fig. S2~~1~~-Fig. S4~~3~~). Overall, bands belonging to sections 1100-1300 nm of the NIR and 2100-2300 of the SWIR regions were rated as the most important bands in PLS. For CP, the red-edge region (680-750 nm) was especially important (Fig. 6~~5.~~). In RF models, the most important bands were located at the visible (400-680 nm), especially those belonging to the green and red sections, and red-edge regions.

Important differences can be observed in the stability of the variables. In PLS models, some variables highly ranked showed low values of stability. That is the case of band 2230, which was the most important band for predicting CP and was selected in only 7% of the times that the backward feature elimination was repeated with bootstrapped data (Fig. 6~~4.~~). On the contrary, band 710, with a lower regression coefficient had a stability value of 85%. For CP using PLS, bands 700 and 710 from red-edge and bands 1160, 1170 and 1180 from NIR were highly stable (Fig. ~~4~~6). In RF the stability of the top-ranked bands is, overall, more in line with their importance value.

3.4. Predictive ability and robustness of PLS and RF models

CP was the variable with the most accurate and stable predictions with both, PLS and RF regressions (~~Fig. 6~~Fig. 7~~.~~). PLS outperformed the predictive ability and robustness of RF for CP and NDF, being the predictive statistics of both methods very similar for ADF and EDOM (~~Fig. 6~~Fig. 7~~.~~). The prediction of CP using PLS showed "good" accuracy ($2 \leq$ RPD< 2.5 and $R^2 \geq 0.7$) with a mean R^2 value of 0.82 and a range of 0.68-0.90. The mean RMSE=2.23% was low and the mean RPD=2.47 with values ranging from 1.81 to 3.23. These statistics were considerably worse when RF was used. RF models to predict CP produced mean R^2 value of 0.68, mean RMSE=3.00% and mean RPD=1.82, indicating "moderate" accuracy ($1.5 \leq$ RPD<2 and $R^2 \geq 0.60$). For NDF, the PLS models had a "moderate" accuracy with mean values of R^2 and RPD 0.62 and 1.71 respectively and mean RMSE=6.05%. However, the accuracy of NDF models dropped to "poor" when the predictions were made with RF, reporting a mean R^2=0.47, mean RPD= 1.41, and mean RMSE=7.20%. For ADF and EDOM, "poor" accuracy was obtained using both PLS and RF since the RMSE was high and mean values of $R^2 < 0.6$ and RPD < 1.5. Only for EDOM predictions with PLS accuracy close to "moderate" was obtained, with mean values of R^2=0.54 and RPD=1.55.

4. Discussion

4.1. Performance of PLS and RF, prediction ability, certainty and backward feature elimination

This study compared two machine learning algorithms widely used in remote sensing, PLS and RF. The results showed that PLS outperformed RF in terms of prediction accuracy and certainty of the predictions of CP and NDF (~~Fig. 6~~Fig. 7). This result differs from several studies reporting higher performance of non-linear algorithms such as Support Vector Machine (SVM), RF or Convolutional neural network (CNN) using hyperspectral data due to their capability to explain complex non-linear relationships in contrast to conventional PLS regression (Pullanagari et al., 2021; Pullanagari et al., 2016; Pullanagari et al., 2018; Ramoelo et al., 2013; Verrelst et al., 2015; Wijesingha et al., 2020; Yao et al., 2015; Zhou et al., 2019). Wijesingha et al. (2020) reported RF outperforming PLS to predict CP and ADF from 194 samples in mountain hay meadows and *Nardus stricta* grasslands using hyperspectral data from UAVs (118 bands of 5 nm spectral resolution, 482–950 nm). However, as Pullanagari et al. (2021) demonstrated using similar data with CNN and PLS, there is a trade off between the number of samples and the performance of the models. In this study, they found that PLS needs a minimum of 200 samples to stabilise the calibration while at least 1500 samples are required for CNN calibration. Little research has been found comparing RF and PLS to predict pasture variables using similar grasslands and comparable hyperspectral canopy reflectance. Further research is needed to explore if the trade off mentioned above between the number of samples and the performance exists comparing RF and PLS regressions.

The results reported on the predictive ability of the models indicate that quantitative predictions of “good” accuracy for CP ($2 \leq$ RPD< 2.5 and $R^2 \geq 0.7$) of Mediterranean permanent grasslands can be achieved using data at a spectral resolution of 10nm. The accuracy drops to “moderate” ($1.5 \leq$ RPD<2 and $R^2 \geq 0.60$) for NDF. Fernández-Habas et al. (2021), also obtained better calibrations for CP and NDF than for ADF and EDOM using Sentinel-2 data to predict pasture quality in Mediterranean permanent grasslands. Therefore, pasture quality maps in Mediterranean grasslands might be based on CP and NDF predictions.

The performance of the models was comparable or even better than results reported from previous studies using similar data. For example, Biewer et al. (2009b) obtained $R^2_{CV} = 0.83$ and RPD=2.4 to predict CP in pure swards and binary legume-grass mixtures using field spectroscopy of spectral resolution 3 nm and 30 nm in the 350-1000 nm region and 1000-2500 nm region respectively. However, the accuracy obtained for ADF (R^2_{CV} = 0.75 and RPD=2) was considerably better than in our case. Safari et al. (2016) obtained worse calibrations for CP than Biewer et al. (2009b), despite using higher spectral resolution which was attributed to the heterogeneity of the grasslands and the reduced spectral range up to 1700 nm. The effect of multiple species composition of grasslands in lower regression accuracy was also pointed out by Kawamura et al. (2008) who reported worse mean R^2=0.62 but lower mean RMSE=1.27 to predict CP. Their results for ADF were slightly better than in this study and worse in the case of NDF. Zhou et al. (2019) reported similar statistics of validation (R^2=0.84) to predict CP in legume and grass mixtures using the 10nm spectral resolution Yara-N sensor by Support Vector Machine, while worse results were obtained by PLS (R^2=0.64). There is still a considerable variation in the accuracy of the results of studies using field spectroscopy to assess pasture quality. The main reasons might be related to variations in sample size and differences in the grasslands assessed (Pullanagari et al., 2012). A key factor that enabled high accuracy to predict CP and NDF in this study is the wide range of the data used to calibrate the models (Table 2), promoted by the heterogeneity and inter-annual variability of Mediterranean grasslands. The growth stage of the grasslands is another factor affecting the canopy reflectance (Zeng and Chen, 2018), and thus the accuracy of the models. In this study, the models have been calibrated using samples from different growth stages and managements to test the accuracy of general models rather than the accuracy of specific models for different growth stages or compositions. Previous studies have investigated the effect of different growth stages and stand mixtures on the estimation of biomass and nutrient contents (Biewer et al., 2009a; Biewer et al., 2009b; Zeng and Chen, 2018; Zhou et al., 2019).

Zeng and Chen (2018) showed differences in reflectance of samples from boot stage, peak growth, and dormancy. However, the PLS models showed improved R^2 from cross-validation and predictions when samples from all three growth stages were combined. Although the reduced number of samples used for the specific growth stages models might have affected the results. They concluded that is feasible to use a model to predict nutrient contents from vegetative to dormancy stages. Biewer et al. (2009a) and Biewer et al. (2009b) reported improved accuracy of predictions of yield and CP by legume-specific calibrations. On the contrary, Zhou et al. (2019) did not find an influence of sites, developmental stage, and species mixtures on the performance of PLS models. Pullanagari et al. (2021) also reported better performance of models using samples from all seasons combined due to a better cover of the variability compared to the season specific models. In agreement with Zhou et al. (2019), we consider that models developed with samples representing different grow stages, managements (grazed or non-grazed) and sites are more generalisable and useful than models calibrated for specific situations. This is especially important in Mediterranean grasslands due to the high heterogeneity promoted by the high species and functional diversity, management, and differing synchrony of growth stages. Thus, specific models might be of limited application in Mediterranean grasslands. As highlighted by Zeng and Chen (2018), the sample diversification of the calibration dataset covering a wide range of situations (phenological stages, sites, management and species composition) is crucial to improve the estimative ability of the models.

Compared to results reported using Sentinel-2 by Fernández-Habas et al. (2021) to predict CP and NDF, the accuracy was improved considerably. This demonstrates that future high-priority mission candidate CHIME (Nieke and Rast, 2018), could improve the quality of the predictions and the retrieval of information from grasslands canopy compared to currently operating multispectral sensors (Berger et al., 2020; Obermeier et al., 2019; Rast et al., 2019; Thenkabail et al., 2000). This improvement in the quality of the predictions is especially important in Mediterranean ecosystems due to the higher heterogeneity of the grasslands (Fava et al., 2009), which demands finer spectral resolution to provide accurate information on the grassland's attributes. However, it has to be considered that the spatial resolution of CHIME (20-30 m) will also play a major role in its potential to monitor grasslands ecosystems (Meier et al., 2020). Here we only tested the spectral resolution, further research involving the spatial resolution is required to get a complete picture of the potential of this promising sensor (Casa et al., 2020). These studies should aim at including the spatial resolution of 20-30 m of the CHIME data in the sampling approach, which together with the results provided in this study could additionally contribute to defining the sources of error and uncertainty of models developed with true CHIME data in the future. Lastly, although the simulation of the spectral resolution of satellites from field spectroscopy has been extensively used in previous research (Adjorlolo et al., 2015; Lugassi et al., 2019; Mutanga et al., 2015; Ramoelo and Cho, 2018; Sibanda et al., 2015), the results obtained from this data must be treated as an approximation to the potential of the future satellite, not as the actual performance of it.

~~Fig. 6~~Fig. 7 illustrates the importance of implementing bootstrap approaches to test the performance and predictive ability of the models. Pullanagari et al. (2021) highlighted the relevance of quantifying and reporting the uncertainty of the predictions as well as using an appropriate sample size. The variation of the models' performance statistics associated with the data partition (~~Fig. 6~~Fig. 7) reveals an inherent uncertainty of the dataset. Reporting information of a single model without testing the certainty of the predictions can lead to biased information (Verrelst et al., 2015). In this study, the interpretation of the model performance was associated with its corresponding uncertainty. This is also relevant when implementing this technology in the management and monitoring of grasslands. It is therefore advisable when reporting information of the predictions, supporting it with the corresponding confidence intervals.

The improvement achieved by the BFE using both algorithms, PLS and RF, is also consistent with previous literature (Mutanga, 2004; Adam et al., 2014; Díaz-Uriarte and Alvarez de Andrés, 2006; Odindi, 2014; Belgiu and Drăgu, 2016; Kawamura et al., 2017; Santos-Rufo et al., 2020). For example, Kawamura et al. (2008) also reported an important decrease of RMSE in cross-validation for CP, NDF and ADF using PLS and 5 nm of spectral resolution of field spectroscopy. The same authors also compared the performance of models using canopy reflectance of the pasture and first derivative reflectance (Kawamura et al., 2008). They found some differences in performance and band selection of models fitted with first derivative reflectance. The spectral preprocessing of the spectra is an interesting topic for future research that, to our knowledge, has not been investigated in deep for pasture quality estimation using field spectroscopy. For example, Dotto et al. (2018) performed a systematic study on 63 spectral preprocessing and multivariate prediction models of soil organic carbon by Vis-NIR spectra using a FieldSpec 3 Spectroradiometer (ASD Inc.). These studies could support choices of spectral preprocessing to improve the prediction capability of the models.

4.2. Importance and stability of bands to predict pasture quality variables

Most of the bands of known absorption features (see Adjorlolo et al. (2013) and Kawamura et al. (2008) for review) or those close to them were selected and highly ranked for the prediction of the corresponding compounds. The results of the bands importance analysis align with results from previous studies highlighting the role of the red-edge region to assess pasture quality due to its relationship to the chlorophyll content of the vegetation (Adjorlolo et al., 2015; Horler, 1983; Kawamura et al., 2008; Ramoelo et al., 2011; Ramoelo and Cho, 2018). Our results showed that this region was commonly selected for all pasture quality variables in both models (~~Fig. 4~~Fig. 5), being also some bands such as band centred at 700 nm highly stable (~~Fig. 5~~Fig. 6). In this study, the 700 nm centred band, ranked second and first in PLS and RF models respectively to predict CP. Adjorlolo et al. (2015) also found the 700 nm waveband as the most important according to the PLS' variable importance projection (VIP) to predict nitrogen content in C3 and C4 grass species. They also found a strong relationship between the 720 nm waveband and CP.- This demonstrates the reliability and importance of ~~this region~~ the red-edge region to assess pasture quality. Bands from NIR and SWIR regions were also commonly selected in PLS and RF for CP and NDF (the best-predicted variables). The selection of bands in these regions lies in the well-known absorption features of cellulose, protein, nitrogen, and starch due to C–H, C–N, N–H, and O–H bonds (Carter, 1994; Clark and Lamb,1991; Curran, 1989; Kawamura et al., 2008; Kokaly, 2001). These results show that a target-oriented selection of bands in these regions can lead to accurate predictions of pasture quality with few bands (Adjorlolo et al., 2015; Kawamura et al., 2008).

The main difference from previous studies is the contrasting selection of bands in the visible region and their importance in RF models compared to PLS models (Fig. 5, Fig. 6, and Fig. S2). The visible region is related to the content of the pigment of vegetation (Blackburn, 1998; Ustin et al., 2009). The pigment content is strongly related to the CP and fibre content, and it is subjected to changes of the phenological stages during the growing season. However, as pointed out by Kattenborn et al. (2019), the up-scaling of pigment concentration to the canopy scale is challenging. Although this trend should be carefully interpreted due to the tendency of RF to select a higher number of bands than PLS by backward feature elimination, one possible explanation for that could lie in the fundamental differences between PLS and RF to model the relationship between predictors and the dependent variable. Since PLS is less suitable for deriving strong non-linear relationships than non-linear models (Pullanagari et al., 2021; Verrelst et al., 2015), RF could better capture the relationships between pigments and canopy reflectance in this region of the spectra. This non-linear relationship between reflectance in the visible range and leaf chlorophyll content has been pointed out in previous research (Blackburn, 1998; Gitelson et al., 2003). For example, Qin (2011) attributed an improved pigments content estimation in grape leaves, using hyperspectral data in the 400-750 nm spectrum, to a non-linear modelling by SVM.

Some of the selected bands showed low stability to the variation of the dataset. This outcome highlights again the importance of testing the uncertainty of the results. The information on the most important bands in these types of studies should be tied to a stability analysis to be more informative. Because of the confounding effect on the reflectance of canopy structure, leaf inclination, plant diversity, plant water content, or different phenological stages (Curran, 1989; Fava et al., 2009; Kattenborn et al., 2019; Pullanagari et al., 2021; Tong and He, 2017; Zhou et al., 2019), the response of the stability of the selected bands in relation to changes in the dataset has important implications to select stable and reliable bands to perform predictions. The stability of band 700 and 710 and 1160-1180 in PLS to predict CP could indicate a strong CP content-reflectance relationship despite the possible cofounding effects mentioned above. However, the bands selected in the region of the spectra from 2000 to 2300 nm reported low stability. This might be caused by the water content of leaves and soil background since Ripple (1986) found the 2080-2350 nm region to be sensitive to both factors. Ramoelo et al. (2011) also highlighted the water effects in the SWIR region for the retrieval of grass nitrogen. In this study, some samples taken in May and June were senescent. The reflectance of senescent grasslands can distinctively show absorption features in the 2006-2196 region of the spectra that otherwise would be masked by the water content in non-senescent grasslands (Mutanga et al., 2004). This can be appreciated in ~~Fig. 4~~Fig. 5 where the reflectance of samples with higher fibre content and lower CP content (senescent conditions), clearly show absorption features in the SWIR region compared to the reflectance of samples with lower fibre content. In RF, the stability was higher, although the considerable number of bands selected might influence that stability measure. Nevertheless, it can be also observed that bands from the SWIR region tend to show lower stability compared to those from the red-edge region. The mix of senescent and non-senescent samples could lead to the lower stability of the SWIR bands in both models. Independent calibration models for different stages could improve the stability of these bands. However, this would reduce the range of the dataset and the generalization of the models since the mix of senescent and non-senescent grasslands is common in Mediterranean grasslands and the transition between both stages is also an important moment to have information about the pasture quality.

4.3. Implication for the management and monitoring of Mediterranean permanent grasslands

PLS models calibrated with the selected bands (from the red-edge and NIR regions) by BFE showed good accuracy in the ~~predictios~~predictions, with high R^2=0.82 and low mean RMSE=2.23%. These results demonstrate that future sensors at this spectral resolution can provide useful information for the management and monitoring of Mediterranean permanent grasslands.

CP content is a crucial attribute of the pasture to inform the management of grasslands and livestock. Having accurate predictions on the content of CP can help the farmers to perform more efficient grazing of Mediterranean grasslands which are subject to high interannual variations of CP. If the predictions can be performed at quantitative level, the utility of the information compared to qualitative predictions increase considerably since it might allow more precise calculation of information such as the carrying capacity of the grasslands or the need and type for supplementary feedstuff for the livestock (Pullanagari et al., 2013; Ramoelo and Cho, 2018; Raab et al., 2020; Starks et al., 2006). If this level of accuracy is achieved with future operational sensors such as CHIME (Nieke and Rast, 2018), this technology might substitute labour manual collection of samples to determine pasture quality (Starks et al., 2004). The difference of precision can be assumed in benefit for spatial predictions acquired on a regular basis in nearly real-time (Pullanagari et al., 2013; Starks et al., 2004). Indeed, pasture quality determination is not frequently performed in farms of Mediterranean permanent grasslands, where the information provided by these determinations might not compensate for the cost of the analysis. Additionally, the delay between manual sampling collection and the reception of the data limits its usefulness since the quality and phenology of Mediterranean grasslands can change rapidly (Pérez-Ramos et al., 2020, Gómez-Giráldez et al. 2020). Therefore, the availability of hyperspectral data can mean a step forward in the adoption of smart farming in Mediterranean grasslands-based farms. However, it has to be considered that a high proportion of Mediterranean grasslands are devoted to traditional small farming (Lowder et al., 2016) for which the implementation of remote sensing technologies might be of limited application and low interest for smallholders.

The analysis of the bands importance and stability to predict the pasture quality indicators has important implications to inform the design of devices aimed at optimising the range of the spectra and the spectral resolution used to assess in-field pasture quality. For example, in the case of CP, it has been demonstrated that field spectrometers with a spectral resolution of 10 nm and 19 target-oriented bands can be sufficient to achieve good accuracy of the predictions.

Finally, the enhanced accuracy provided by forthcoming CHIME in combination with currently operating services such as Sentinel-2 opens new opportunities to monitor Mediterranean grasslands ecosystems in the context of the next renewal of the Common Agricultural Policy (CAP) (Rast et al., 2019). This technology can be used to assess the compliance of the CAP and Natura 2000 regulations and the conservation status of grasslands ecosystems at the national scale (Griffiths et al., 2020).

5. Conclusion

Concerning the objectives of the study the conclusions are:

i) Hyperspectral narrow bands from field spectroscopy at 10 nm of spectral resolution CHIME-like show potential to predict CP at good accuracy and NDF at moderate accuracy level in Mediterranean permanent grasslands. ADF and EDOM were predicted with poor accuracy.

ii) PLS outperformed RF to predict CP and NDF in terms of accuracy and certainty of the predictions.

iii) BFE can considerably reduce the number of bands used in the predictions while improving the accuracy of the models, especially in PLS regressions.

iv) Bands from the red-edge and NIR regions show high importance and stability to assess the best-predicted variables. Bands centred at 700, 710, 1160, 1170 and 1180 are highly stable and important to predict CP. The bands belonging to the SWIR region show lower stability.

v) These results prove the potential of hyperspectral data and future satellite missions such as CHIME to inform the management and monitoring of Mediterranean permanent grasslands.

Further research needs to be carried out to advance towards the applicability of the results here reported to practical farming in Mediterranean permanent grasslands.

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Table 1. Grassland type, number of samples and date of sampling of the farms used in the study.

Farm	Coordinates*	Grassland type	Sampling date		Number of samples
1	x= 315534.34 y= 4263109.14	Permanent natural grasslands	2012/2013	January/ February March April May June	28
2	x= 350946.02 y= 4244905.06	Permanent natural grasslands	2012/2013	January/ February March April May June	33
3	x= 352598.98 y= 4235836.66	Permanent natural grasslands	2012/2013	January/ February March April May June	33
4	x= 387377.62 y= 4230454.12	Permanent natural grasslands	2012/2013	January/ February March April May June	31
5	x= 331065.33 y= 4197542.60	Permanent natural grasslands	2018/2019	May	12
		Reseeded grasslands			24
		Irrigated grasslands			12
				Total samples	173

*Projected coordinate system: ETRS 1989 UTM Zone 30N

Table 2. Descriptive statistics of the pasture quality variables used to fit the models.

Pasture variables (% of DM)	Minimum	Mean	Maximum	Range	SD	CV
CP	3.7	11.9	27.7	24.0	5.4	45.4
NDF	24.9	52.0	71.3	46.5	10.1	19.4
ADF	15.7	31.8	44.8	29.1	6.2	19.4
EDOM	38.5	58.4	86.2	47.8	10.8	18.4

CP: crude protein; NDF: neutral detergent fibre; ADF: acid detergent fibre; EDOM: enzyme digestibility of organic matter; SD: standard deviation; CV: coefficient of variation.

Table 3. Performance of PLS and RF models with all bands and with selected bands. Coefficient of determination R^2 and root mean square error (RMSE) correspond to leave-one-out and out-of-bag estimations for PLS and RF respectively.

Pasture variables (% of DM)	Model	All bands			Selected bands					
		NLV	R^2	RMSE	NLV	R^2	RMSE	NBS	%BS	ΔRMSE
CP	PLS	11	0.79	2.48	11	0.84	2.17	21	12.5	-12.5
	RF	-	0.70	2.95	-	0.71	2.89	55	32.7	-2.0
NDF	PLS	11	0.60	6.34	10	0.67	5.77	26	15.5	-9.0
	RF	-	0.52	6.98	-	0.53	6.86	82	48.8	-1.7
ADF	PLS	3	0.40	4.74	6	0.46	4.52	7	4.2	-4.6
	RF	-	0.42	4.68	-	0.45	4.55	53	31.5	-2.8
EDOM	PLS	9	0.53	7.35	6	0.59	6.89	17	10.1	-6.3
	RF	-	0.47	7.83	-	0.51	7.52	34	20.2	-4.0

N=164; NBS: number of bands selected by backward feature elimination; %BS: percentage of bands selected from the original dataset (n=168); ΔRMSE: decrease in root mean squared error from model with all bands to models with selected bands. CP: crude protein; NDF: neutral detergent fibre; ADF: acid detergent fibre; EDOM: enzyme digestibility of organic matter

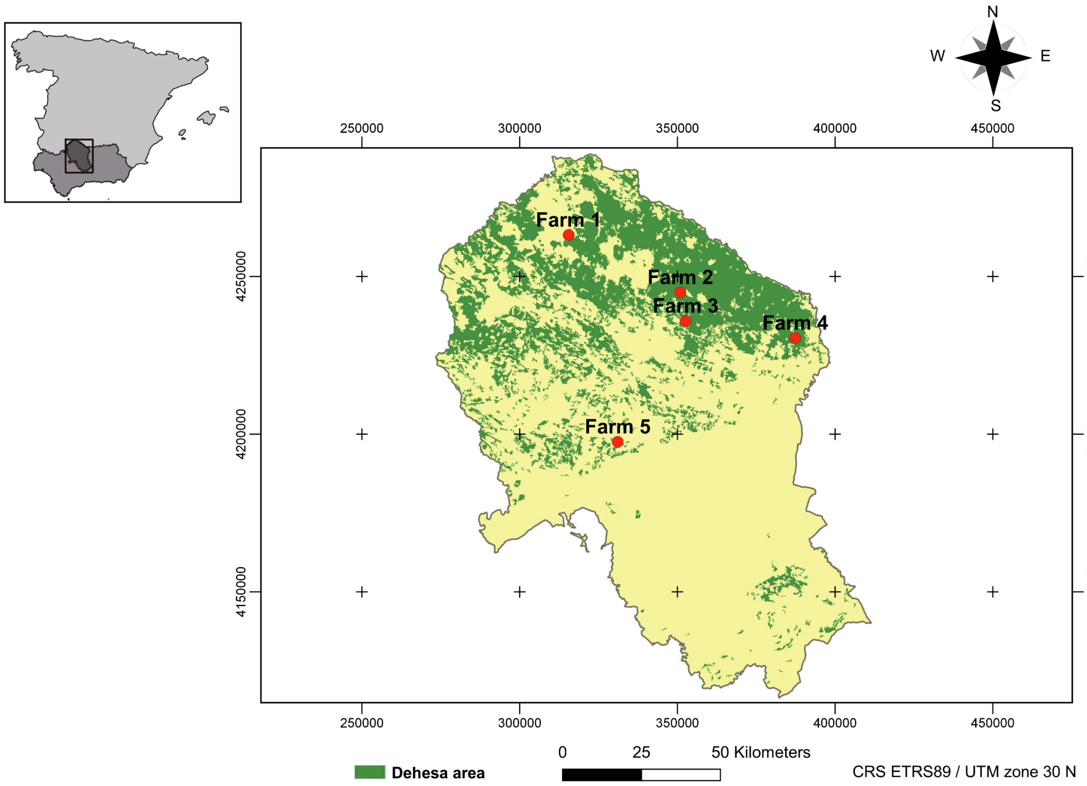

Fig. 1. Location of farms where the grasslands samplings were performed. Farms are located within the *Dehesa* area of Cordoba province, in the north of Andalusia region (Spain). *Dehesa* area layer, coloured in green, is provided by the WMS of the *Dehesa* systems distribution in Andalusia (REDIAM, 2020).

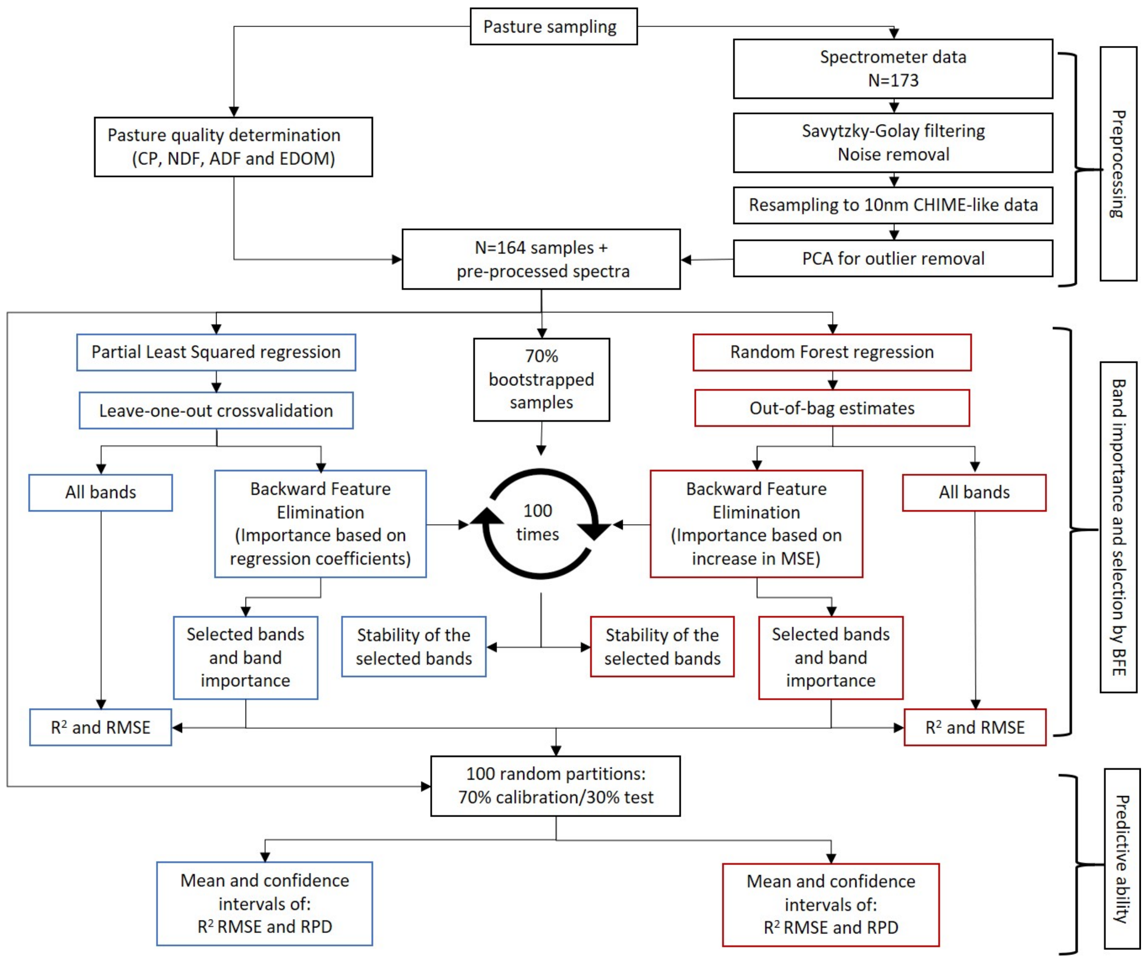

Fig. 2. Modelling approach of the study.

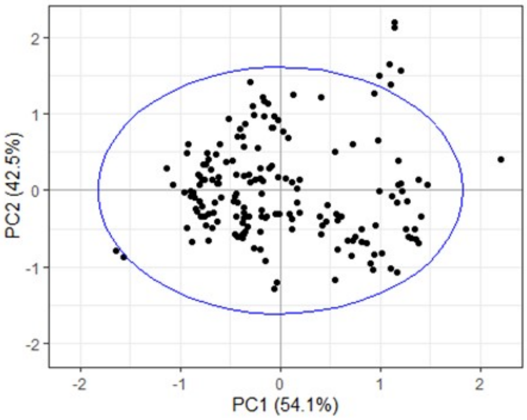

Fig. 3. Detection of outliers after principal component analysis (PCA) of the pasture samples (n=173). Blue line represents 95% confidence ellipse.

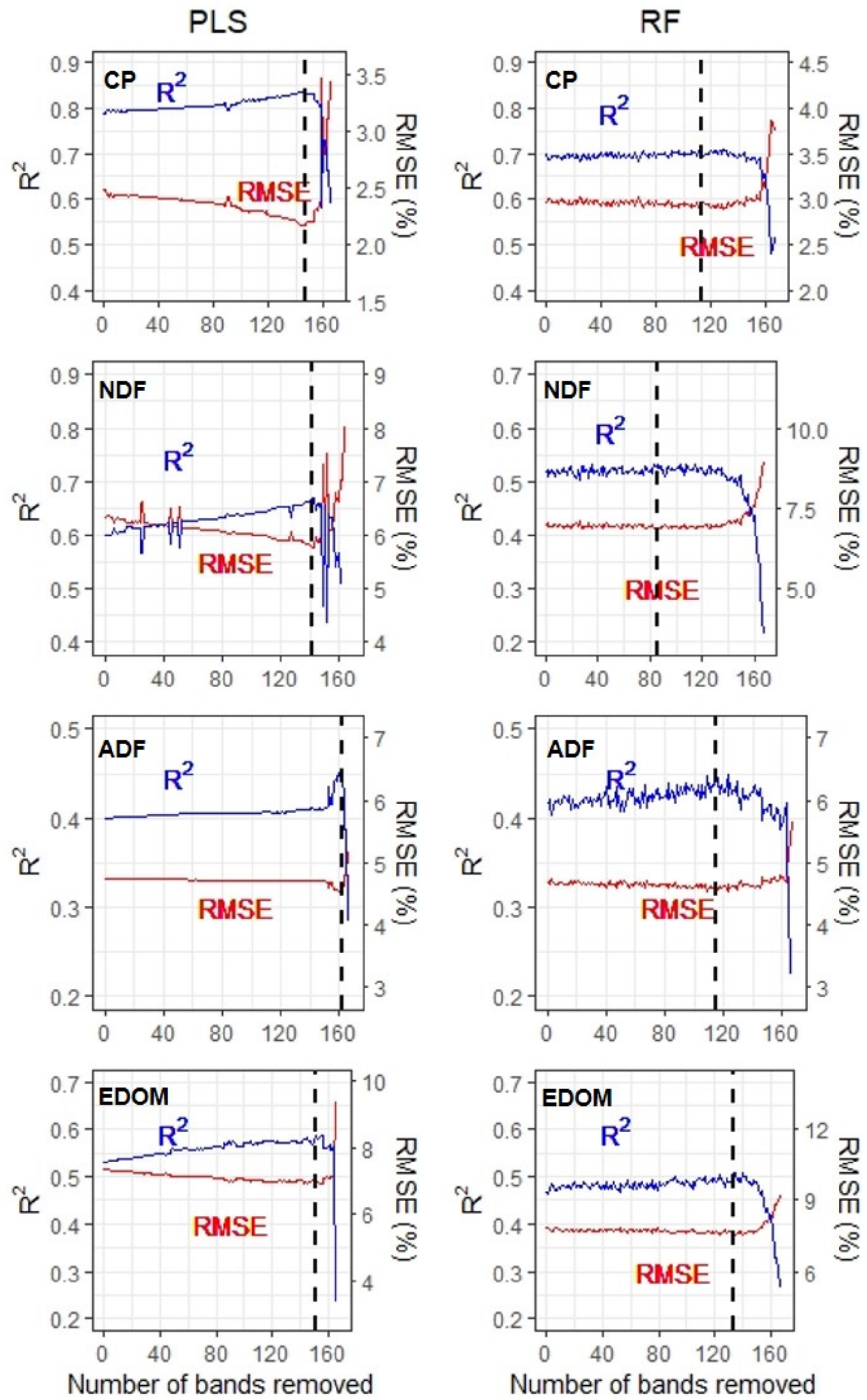

Fig. 4. Changes of R^2 and RMSE in backward feature elimination of redundant bands using PLS (leave-one-out estimations) and RF (out-of-bag estimations) regressions for crude protein (CP), neutral detergent fibre (NDF), acid detergent fibre (ADF), and enzyme digestibility of organic matter (EDOM) (n=164). Dashed lines indicate the minimum RMSE value and maximum R^2 at which the optimal number of bands is reached.

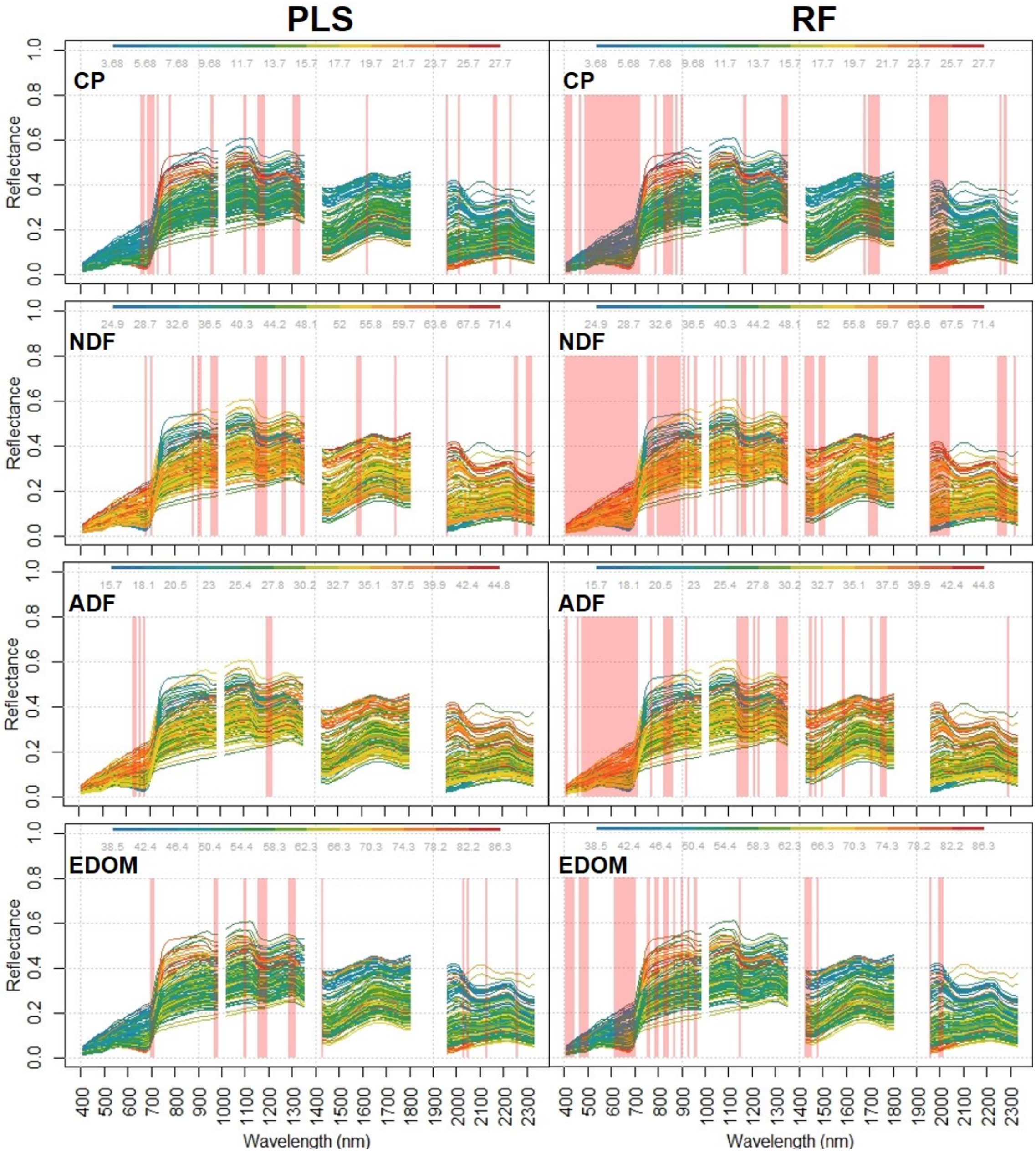

Fig. 5. Canopy reflectance of the pasture samples (n=164) coloured by the content of the respective pasture quality variable: crude protein (CP); neutral detergent fibre (NDF); acid detergent fibre (ADF); and enzyme digestibility of organic matter (EDOM). Vertical red lines indicate the selected bands by backward stepwise feature elimination using PLS (left) and RF (right).

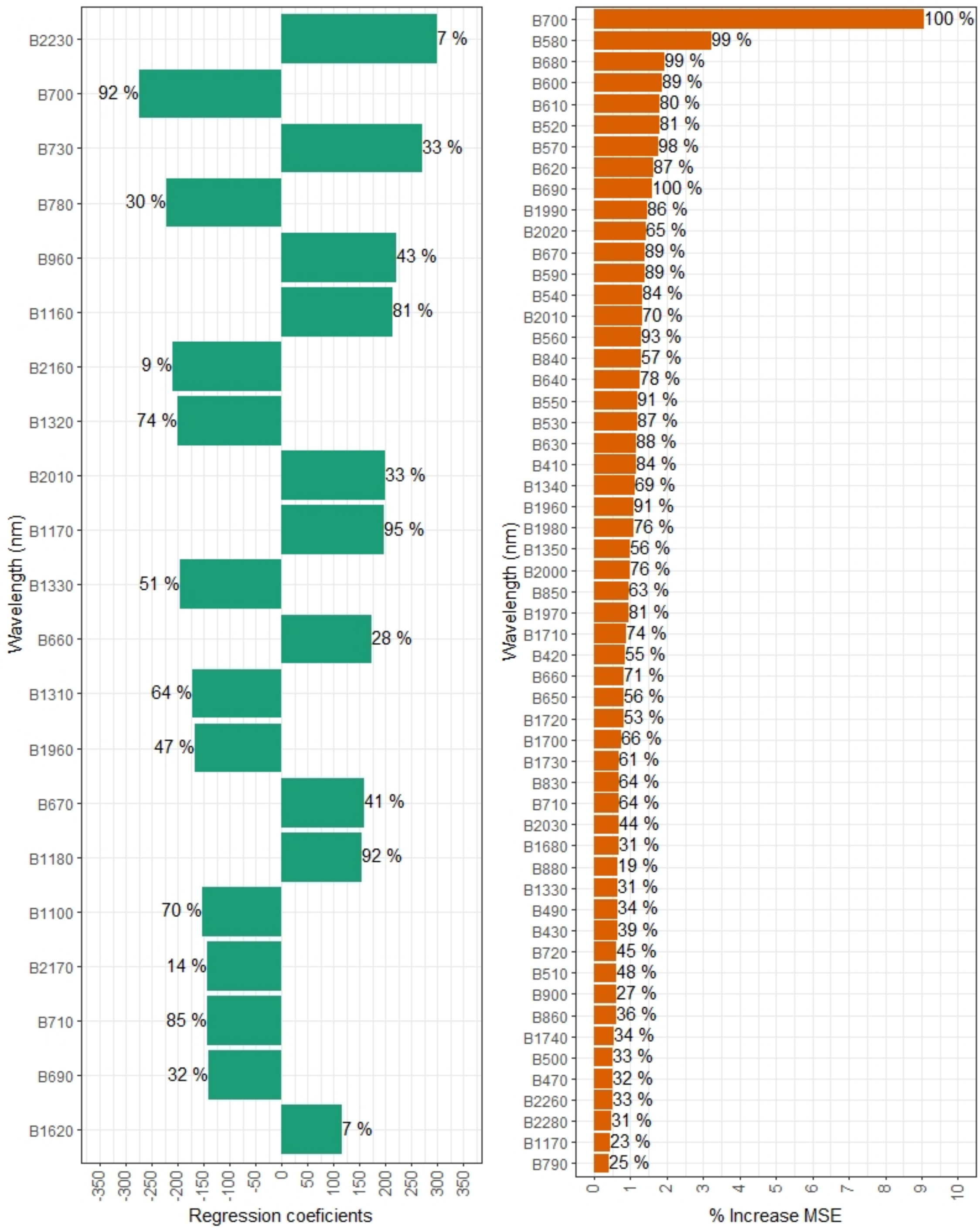

Fig. 6. Importance and stability of selected bands for crude protein (CP) by backward stepwise feature elimination with PLS (21 bands) and RF (55 bands). Importance is measured in absolute value of the regression coefficients of selected bands in PLs and in % increase of mean squared error (MSE) in RF. Stability is indicated as % times the bands were selected in 100 repetitions of the backward feature elimination with using 70% of the samples each time selected by bootstrap with replacement.

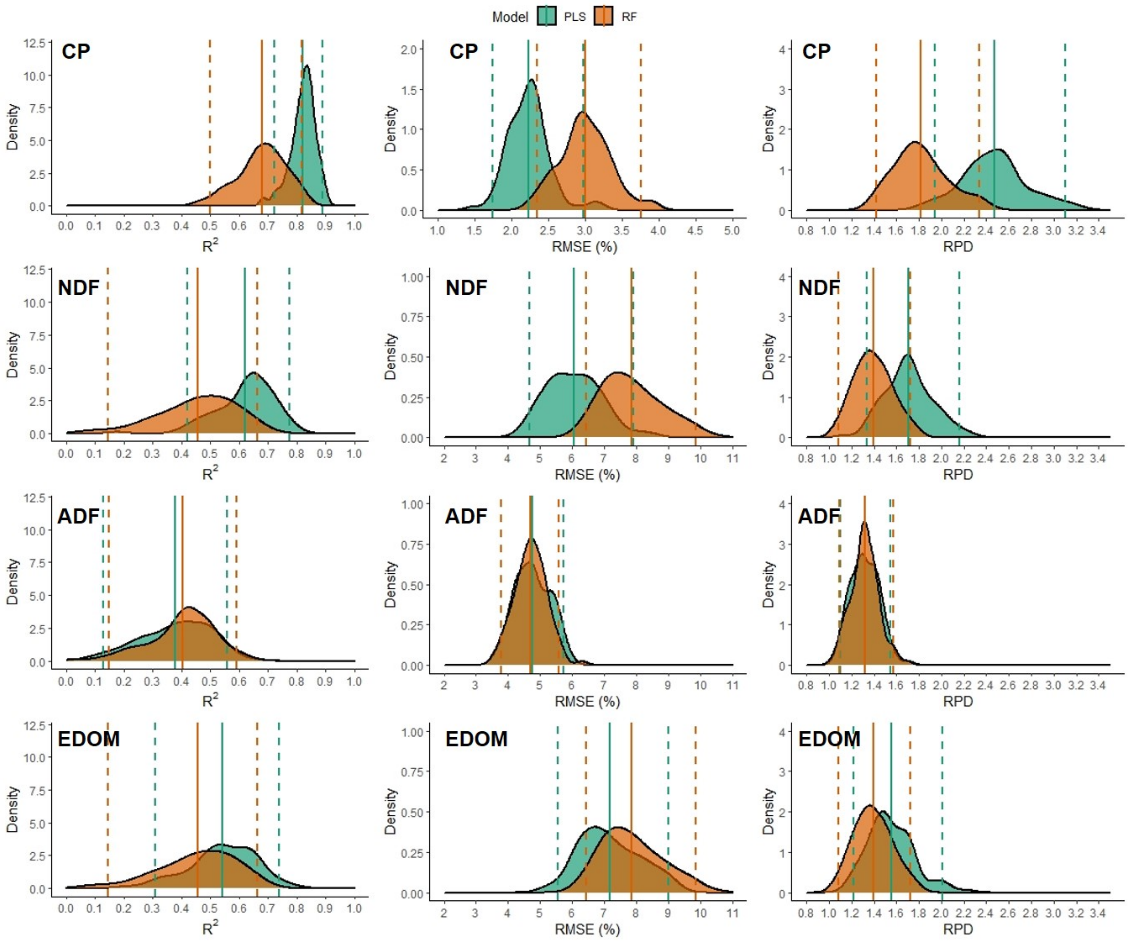

Fig. 7. Density distribution of values of R^2, root mean square error (RMSE %) and ratio of predicted deviation (RPD) from predictions over 30% of bootstrapped samples using PLS and RF models. Calculated from n=100 random partitions of the dataset (n=164) into 70% for calibration and 30% for test with replacement. The predicted parameters are; crude protein (CP); neutral detergent fibre (NDF); acid detergent fibre (ADF); and enzyme digestibility of organic matter (EDOM). Solid lines show the mean and dashed lines show the confidence intervals (2.5 and 97.5 percentiles).

Estimating pasture quality of Mediterranean grasslands using hyperspectral narrow bands from field spectroscopy by Random Forest and PLS regressions

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Supplementary material

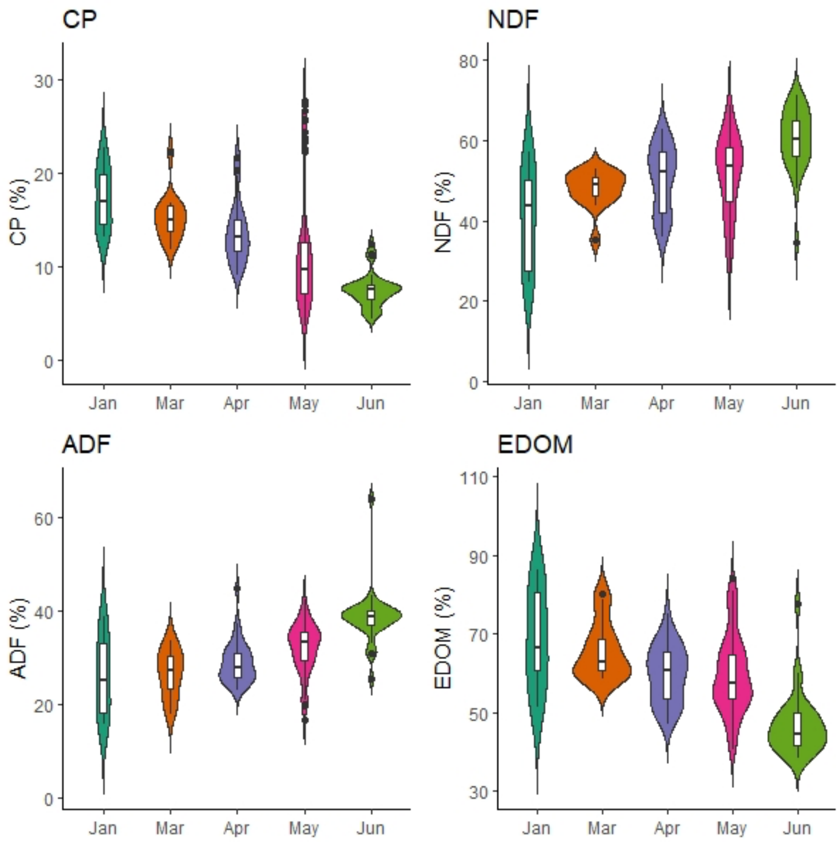

Fig. S1. Variation of pasture quality variables used to fit the models (N=164) by month. Black centre line, median; box, interquartile range; box limits, lower and upper quartiles; whiskers, 1.5× interquartile range; points, outliers. Coloured area indicates the sample distribution. *May includes samples from 2013 and 2019. CP: crude protein; NDF: neutral detergent fibre; ADF: acid detergent fibre; and EDOM: enzyme digestibility of organic matter.

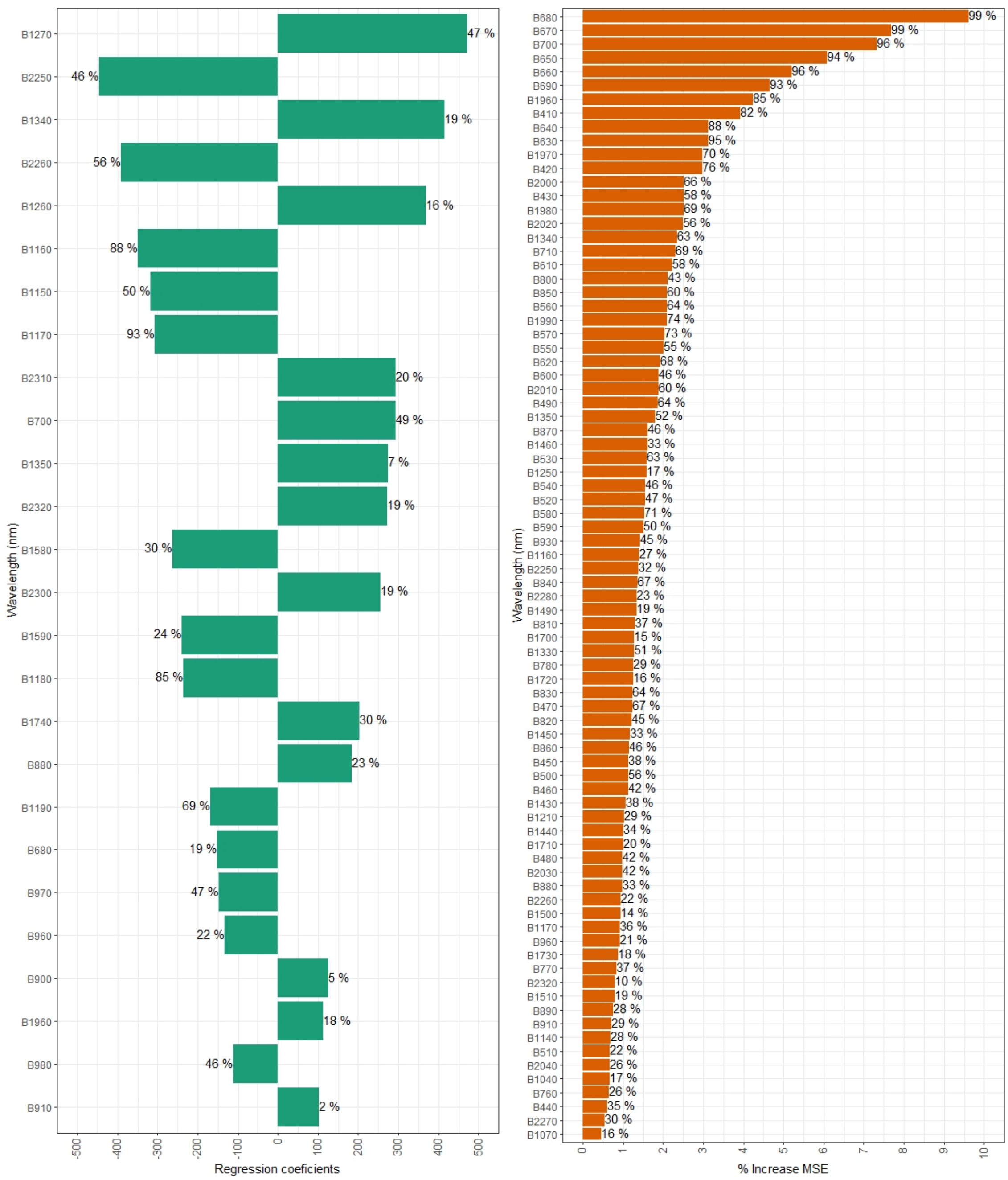

Fig. S2. Importance and stability of selected bands for neutral detergent fibre (NDF) by backward stepwise feature elimination with PLS (21 bands) and RF (55 bands). Importance is measured in the absolute value of the regression coefficients of selected bands in PLs and in % increase of mean squared error (MSE) in RF. Stability is indicated as % of times the bands were selected in 100 repetitions of the backward feature elimination with using 70% of the samples each time selected by bootstrap with replacement.

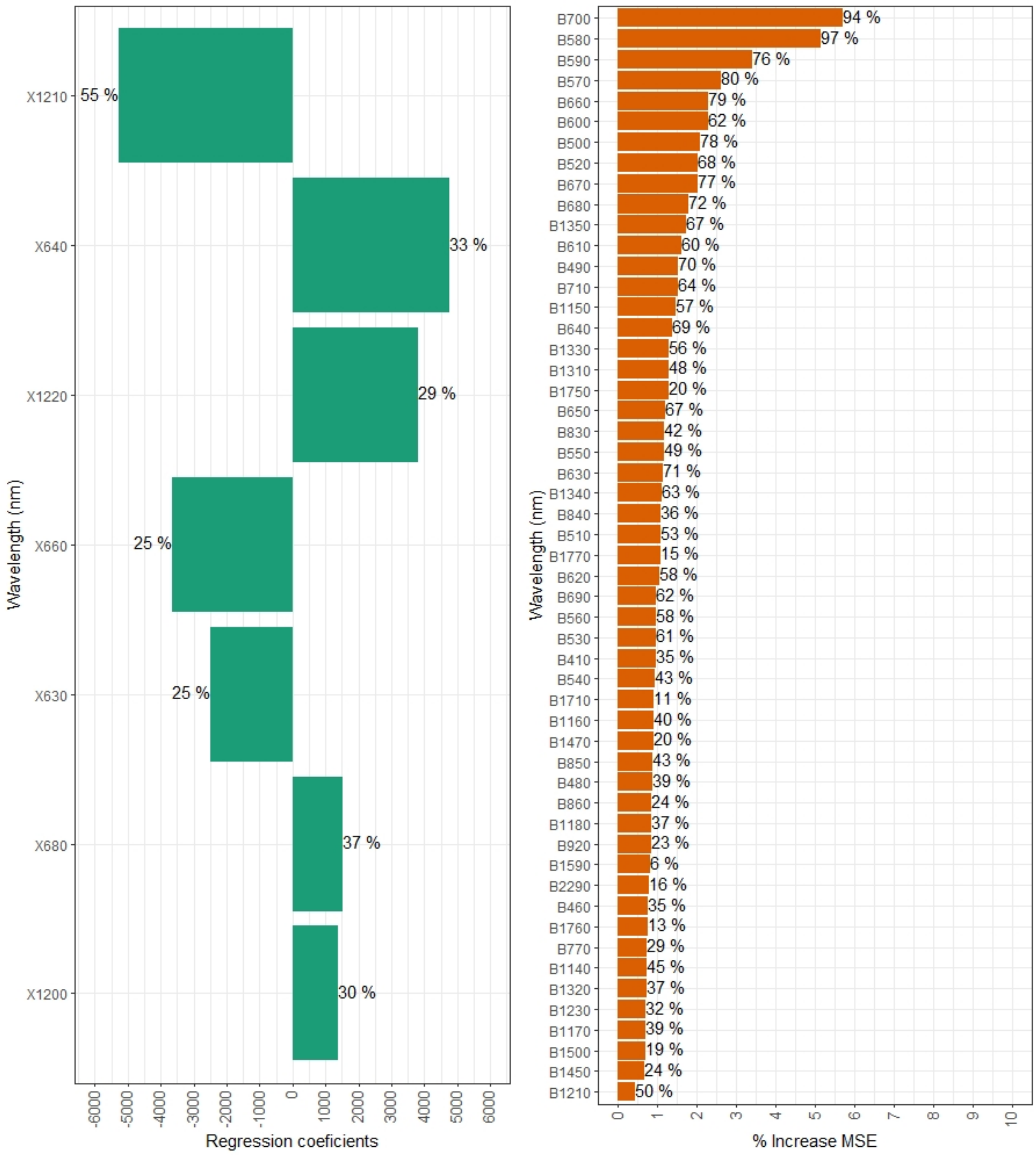

Fig. S3. Importance and stability of selected bands for acid detergent fibre (ADF) by backward stepwise feature elimination with PLS (21 bands) and RF (55 bands). Importance is measured in the absolute value of the regression coefficients of selected bands in PLs and in % increase of mean squared error (MSE) in RF. Stability is indicated as % of times the bands were selected in 100 repetitions of the backward feature elimination with using 70% of the samples each time selected by bootstrap with replacement.

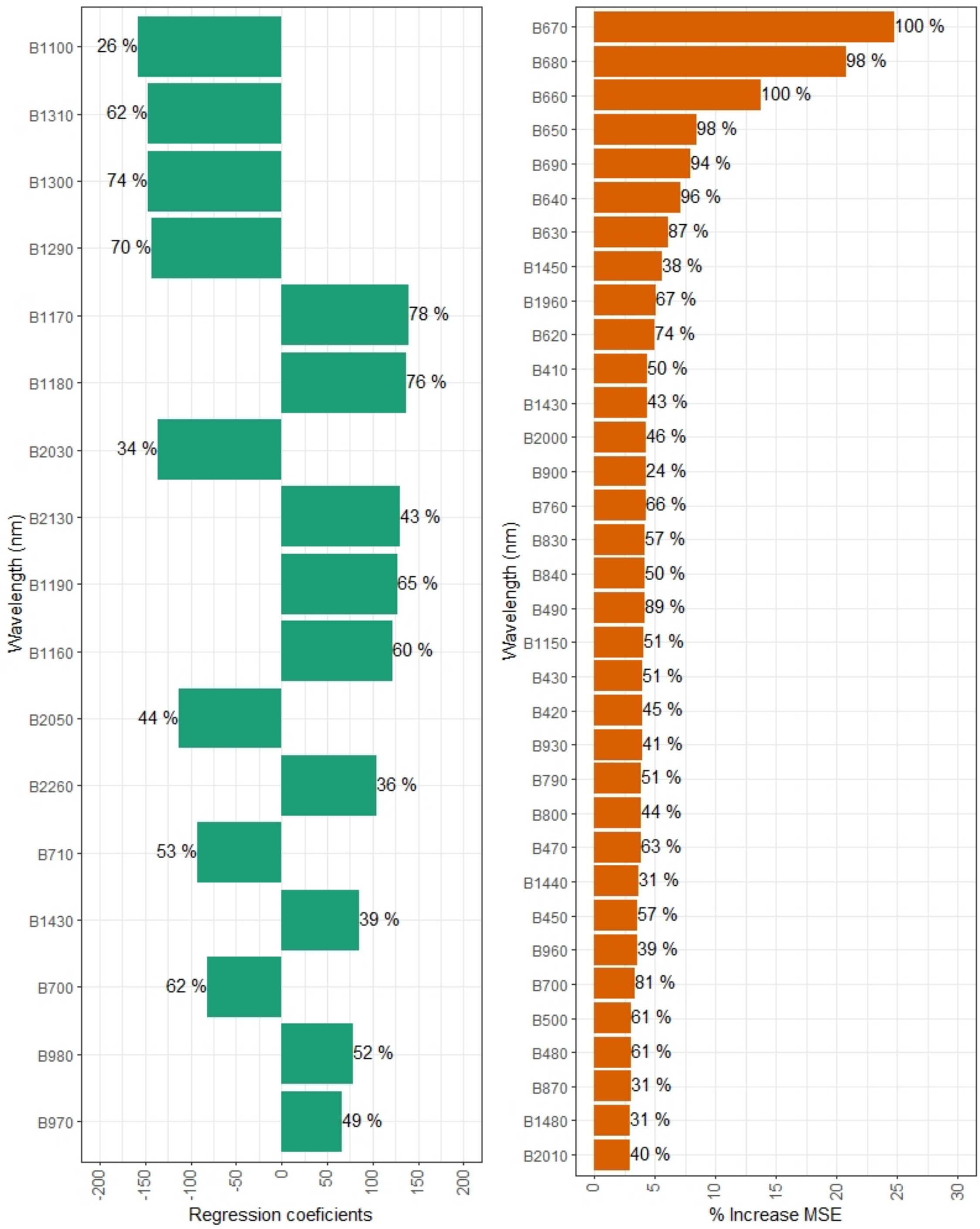

Fig. S4. Importance and stability of selected bands for enzyme digestibility of organic matter (EDOM) by backward stepwise feature elimination with PLS (21 bands) and RF (55 bands). Importance is measured in the absolute value of the regression coefficients of selected bands in PLs and in % increase of mean squared error (MSE) in RF. Stability is indicated as % of times the bands were selected in 100 repetitions of the backward feature elimination with using 70% of the samples each time selected by bootstrap with replacement.

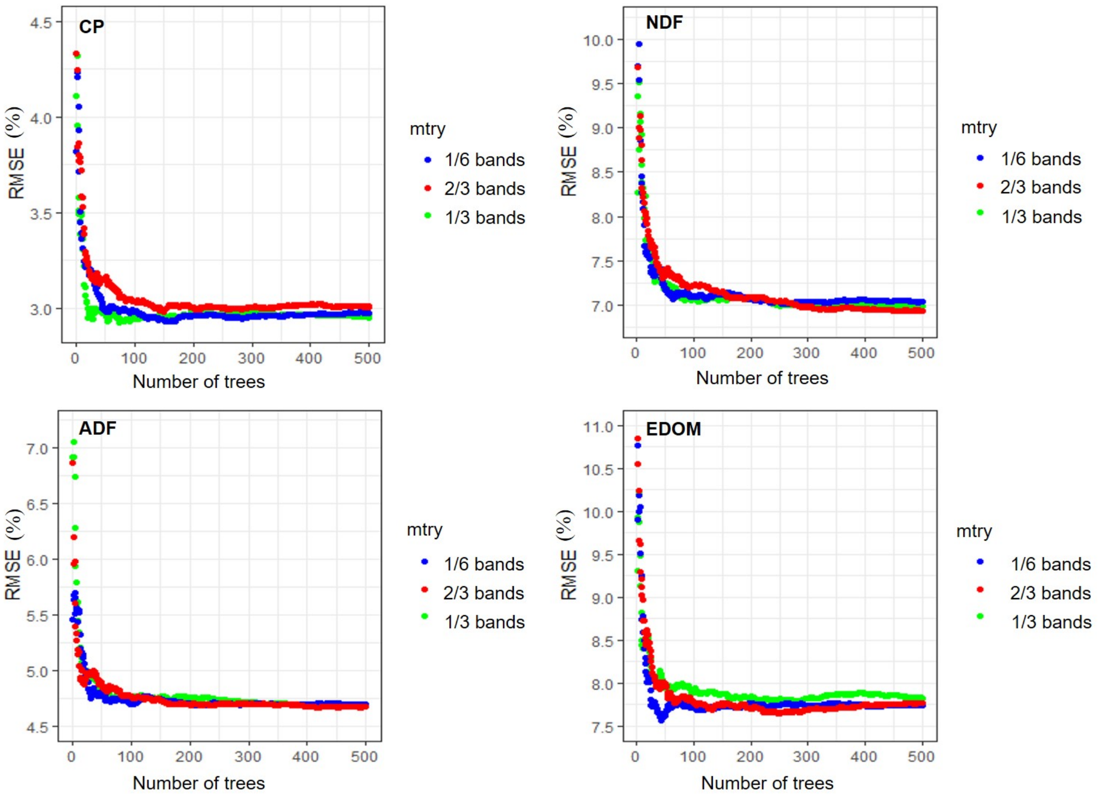

Fig. S5. Changes in RMSE of RF models using all bands for each pasture quality variable with different mtry and ntree values. Default settings are mtry=1/3 and ntree=500. CP: crude protein; NDF: neutral detergent fibre; ADF: acid detergent fibre; and EDOM: enzyme digestibility of organic matter.

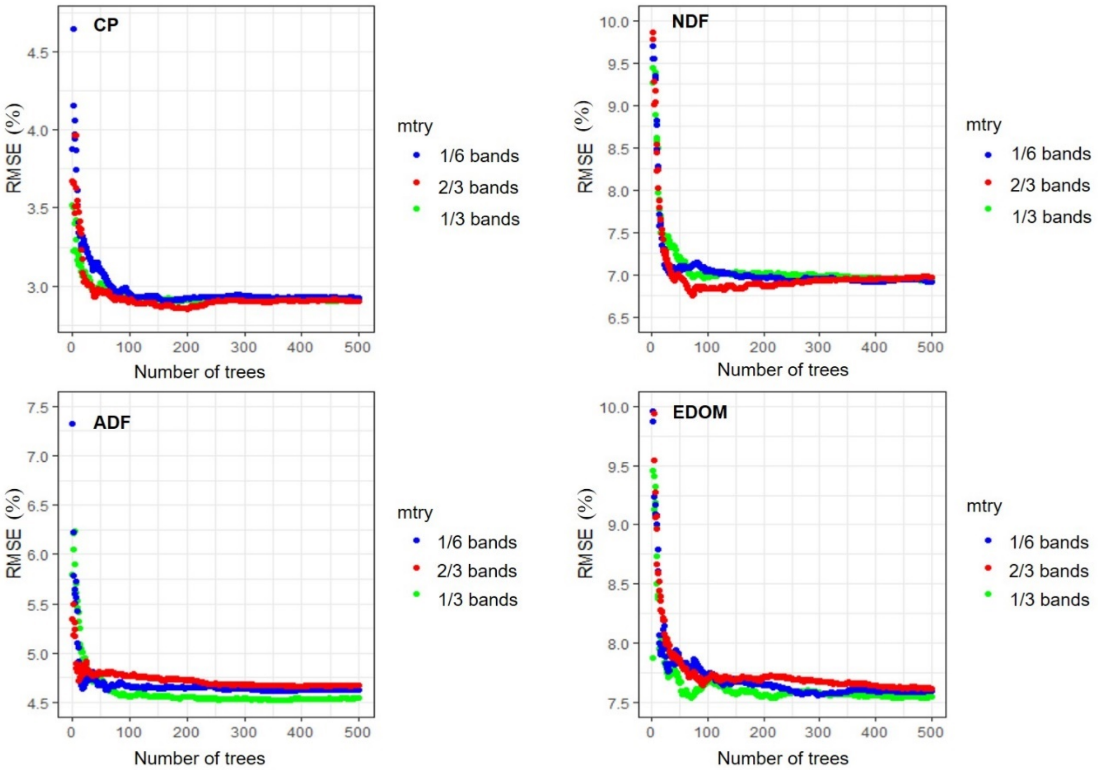

Fig. S6. Changes in RMSE of RF models using the selected bands for each pasture quality variable with different mtry and ntree values. Default settings are mtry=1/3 and ntree=500. CP: crude protein; NDF: neutral detergent fibre; ADF: acid detergent fibre; and EDOM: enzyme digestibility of organic matter.