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Nonlinear parametric modelling to study how soil properties affect crop yields and NDVI

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Abstract

This paper explores the use of a novel nonlinear parametric modelling technique based on a Volterra Non-linear Regressive with eXogenous inputs (VNRX) method to quantify the individual, interaction and overall contributions of six soil properties on crop yield and normalised difference vegetation index (NDVI). The proposed technique has been applied on high sampling resolution data of soil total nitrogen (TN) in %, total carbon (TC) in %, potassium (K) in cmol kg^{-1}, pH, phosphorous (P) in mg kg^{-1} and moisture content (MC) in %, collected with an on-line visible and near infrared (VIS-NIR) spectroscopy sensor from a 18 ha field in Bedfordshire, UK over 2013 (wheat) and 2015 (spring barley) cropping seasons. The on-line soil data were first subjected to a raster analysis to produce a common 5 m by 5 m grid, before they were used as inputs into the VNRX model, whereas crop yield and NDVI represented system outputs. Results revealed that the largest contributions commonly observed for both yield and NDVI were from K, P and TC. The highest sum of the error reduction ratio (SERR) of 48.59% was calculated with the VNRX model for NDVI, which was in line with the highest correlation coefficient (*r*) of 0.71 found between measured and predicted NDVI. However, on-line measured soil properties led to larger contributions to early measured NDVI than to a late measurement in the growing season. The performance of the VNRX model was better for NDVI than for yield, which was attributed to the exclusion of the influence of crop diseases, appearing at late growing stages. It was recommended to adopt the VNRX method for quantifying the contribution of on-line collected soil properties to crop NDVI and yield. However, it is important for future work to include additional soil properties and to account for other factors affecting crop growth and yield, to improve the performance of the VNRX model.

Keywords

Yield limiting factors; proximal soil sensing; nonlinear parametric modelling; VNRX.

1. Introduction

Increasing crop yields requires the precision management of external farm resources (i.e., agrochemicals and fertilisers), which will help reduce input costs and detrimental environmental impacts. Precision management of farm resources requires an understanding and quantification of factors that limit crop yields, which is a research question yet to be comprehensively answered. This currently prohibits precision management of farm resources to be a routine activity. However, precision management of farm resources to correct existing yield limiting factors require high sampling resolution data of variables impacting crop growth and yield, which can then be incorporated within an analytical system. To realise this, robust and reliable sensing platforms for soil and crop are needed. Due to the complexity and high spatial variability of soils, the application of proximal soil sensors is still under active research. Kuang et al. (2012) argue that the most favourable methods for on-line measurement of key soil properties are visible and near infrared (VIS-NIR) spectroscopy and electrochemical methods. The former is based on diffuse reflectance light collected from a soil surface subjected to an external light source, whereas the latter uses ion selective elements to produce a voltage output in a solution in response to the activity of the selected ion (e.g., hydrogen, nitrate). Whilst VIS-NIR is most appropriate to soil properties have direct spectral responses in the NIR spectral range, i.e., organic carbon (OC), moisture content (MC), clay and clay mineralogy (Stenberg et al., 2010), electrochemical methods are capable of quantifying mobile elements i.e., nutrients, mineral nitrogen, or pH (Adamchuk et al., 1999). Since a soil solution is required for electrochemical sensors, their on-line use is impeded. Although on-line VIS-NIR spectroscopy sensors are capable of collecting high sampling resolution data (e.g., >500 samples per ha), they are limited to few research groups (Christy, 2008; Shibusawa, et al. 2001; Mouazen et al., 2006a). Once key soil properties needed in the analytical system are successfully collated using an on-line sensor, information about crop growth (i.e., normalised difference vegetation index (NDVI) or leaf area index (LAI)) can be obtained at high sampling resolution by means of earth observation utilising satellite, airborne, drones or proximal crop sensing platforms.

Previous research has often assumed that the relationship between crop yield and growth limiting factors is linear or approximately linear, which could be untrue for typically complex agriculture systems. Mitscherlich (1909) proposed a model that simulates crop response to growth factors increase. The model assumes that yield potential is constant, and isn’t affected by other factors that limit actual yields under field conditions; a further assumption that may be false in complex agricultural systems. To reveal and characterise information hidden within this complex system, a non-linear modelling approach is required to describe the dependence among soil properties, NDVI and crop yield. Through these means, yield limiting soil properties can be quantified.

Nonlinear methods include, among others, non-linear regression analyses and machine learning. The Nonlinear Auto-Regressive Moving Average Model with eXogenous inputs (NARMAX) is a parametric modelling method introduced by Billings et al. (1989). It is a popular class of nonlinear system identification methods for a complex system, which represents a typical input-output system with an unknown inner structure. Compared to machine learning methods, an advantage of NARMAX is transparency. This means it can be written down and easily understood and interpreted, related to known and existing models, as well as being coupled with frequency domain or statistical analyses. These characteristics are attractive for studying brain climatic change and agriculture systems that are typical input-output systems with unknown inner structures. A Volterra Nonlinear Regressive with eXogenous inputs (VNRX) is a special case of NARMAX that has more recently been introduced. Although VNRX has had successful applications in brain signal analysis (Sarrigiannis et al., 2014; Zhao et al., 2012), climate change (Bigg et al., 2014; Zhao et al.,

2016) and non-destructive tests (Zhao et al., 2017), its application in agriculture is novel due to its capability to reveal hidden nonlinear information while other modelling methods cannot. To our best knowledge no literature about the use of the VNRX model to predict NDVI and crop yield based on on-line measured soil properties is available. This is important to investigate, since on-line soil sensors provide high sampling resolution data (>500 sample per ha), to enable accounting for variability over small spatial scales (e.g., few meters), which cannot be efficiently achieved using traditional methods of soil sampling and laboratory analyses that are tedious, time consuming and costly.

This study's aim is to implement a novel parametric VNRX model to quantify individual, interaction and collective contribution of six soil properties (i.e., TN, total carbon (TC), potassium (K), pH, phosphorous (P), and MC) on crop yield and NDVI. Soil data has been collected at a high sampling resolution with an on-line VIS-NIR spectroscopy sensor.

2. Materials and methods

2.1 Study site and data collection

The study site is located on commercial farmland in Wilstead, Bedfordshire, United Kingdom at coordinates 52°6'0.00"W latitude and 0°26'42.00"N longitude. The field is approximately 18 ha in area, with an average annual rainfall of 598 mm. The farms crop rotation consists of barley, wheat and oil seed rape. The representative soil texture across the field to a depth of 0.20 m is non-homogeneous, including three textures of sandy loam, loam and sandy clay loam in accordance with the United States Department of Agriculture (USDA) texture classification system (Soil Survey Staff, 1999). Wheat and spring barley were cultivated over the experiment timescale during the 2013 and 2015 cropping seasons, respectively. Soil properties, yield and NDVI data were collected using an on-line VIS-NIR spectroscopy sensor (Mouazen, 2006), on-board yield sensor from the farmer's combine harvester (New Holland, CX8070 model), and a Crop Circle sensor (Crop Circle ACS 470, Holland Scientific, Lincoln, NE USA), respectively. Wheat NDVI was measured in the booting (growth stage 43) and heading (growth stage 52) stages, in May and June 2013, respectively. Spring barley NDVI was measured during the stem extension (growth stage 37) and booting (growth stage 43) stages in April and May 2015, respectively. The growing stages are determined in accordance with Zadok's decimal growth scale (Zadoks et al., 1974).

The on-line VIS-NIR soil sensor (Mouazen, 2006b) (Fig. 1) consisted of an AgroSpec mobile, VIS-NIR spectrophotometer (tec5 Technology for Spectroscopy, Germany), with a measurement range of 305-2200 nm. It has a differential global positioning system (DGPS) (EZ-Guide 250, Trimble, USA) to record the position of the on-line measured spectra with sub-metre accuracy. An optical probe fitted behind a subsoiler collected diffuse reflected

Fig. 1. The tractor mounted on-line visible and near infrared (VIS-NIR) spectroscopy sensor (Mouazen, 2006b).

spectra from the bottom of a smooth soil trench formed by the subsoiler. A 20 W halogen lamp supplied by a tractor battery illuminated the base of the trench with artificial light. A semi-rugged laptop was used for data logging and communication to the instrument.

On-line soil measurements were carried out in September 2012 and 2014, following crop harvest, using the method reported in Mouazen et al. (2005). These measurements will be referred to as 2013 and 2015 soil measurements, respectively, throughout the manuscript. The on-line sensor produced measurement transects that were 6 cm wide, 15 cm deep, and were distanced 15 m apart. The spectral measurements were collected with an average forward speed of 2 km h^{-1}. Both on-line measurement and collection of soil samples were performed prior to seed drilling (October in 2012 for wheat and February 2015 for spring barley) and fertilisation (April to June in 2013 and 2015). Soil property changes during winter between on-line measurement and next growing season are minimal, except for MC. However, the spatial distribution of MC in a topographically uniform field like the study site may be similar to the spatial distribution of clay (Mouazen et al., 2014), suggesting that the general spatial pattern of MC would not significantly change from year to year. Only nitrogen fertiliser was homogeneously applied in the 2013 and 2015 cropping seasons, whereas no K or P fertilisers were applied.

2.2 Laboratory analysis and development of calibration models of soil properties

Ten soil samples per hectare (183 samples per 18 ha field area) based on a 30 by 30 m grid (Fig. 2) were collected during the on-line measurement in 2012 from the bottom of the subsoiler trenches. Sampling positions were recorded with a DGPS (Shaddad et al., 2016). Approximately 700 g representing each soil sample was prepared as a composite of soil collected over a 1.5 m travel distance at about 0.15 m depth. Soil samples were placed into tightly sealed plastic bags to hold field moisture, and kept refrigerated at 4 ºC, until

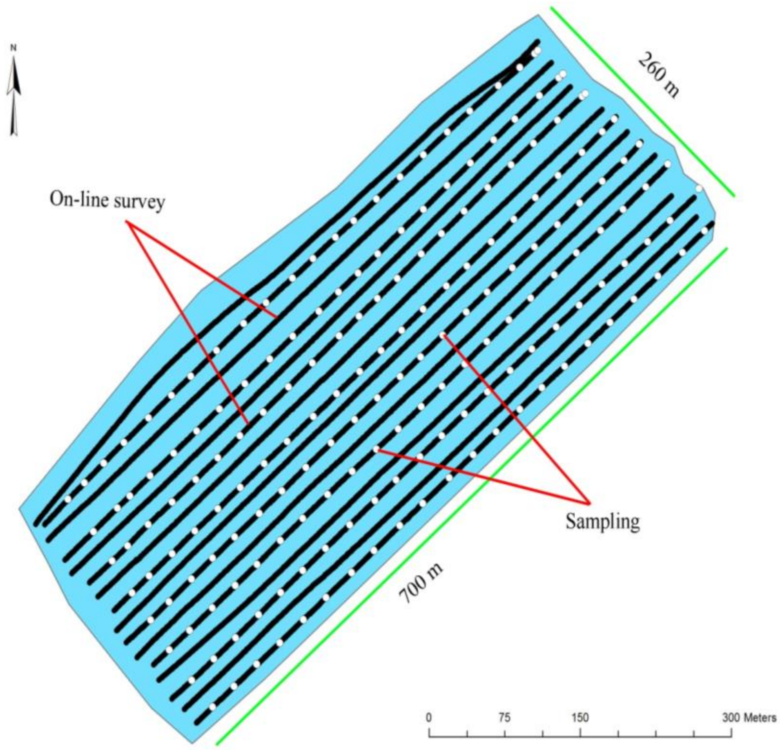


Fig. 2. On-line field survey transects and locations of 183 soil samples (Shaddad et al., 2016).

laboratory analyses to determine TN, TC, K, pH, P and MC. These analyses were based on the following procedures:

- TN and TC were determined with CHN 628 elemental analysis by combustion (LECO, USA) (British Standard Institute, 1995).
- Exchangeable K was determined using an atomic absorption spectrometer (AA analyst 200 Perkin Elmer Instruments, Shelton, Connecticut, USA).
- pH was measured using a glass electrode in a 1:5 (volume fraction) suspension of soil in distilled water (British Standard Institute, 1998).
- Extractable P was obtained in sodium hydrogen carbonate solution according to ISO 11263:1994 (Olsen et al., 1954) and was determined by colorimetric approach using UV-VIS-NIR spectrophotometer (Murphy and Riley, 1962).
- Gravimetric MC was measured with oven drying at 105 ºC for 24 h (British Standards Institute, 2007).

Results of laboratory analyses and spectral measurements were pooled together in one matrix. The 183 soil samples were randomly split into calibration (70% of samples) and validation (30%) sets. The calibration set was subjected to partial least squares regression (PLSR) analysis to establish calibration models for the studied soil properties using Unscrambler V9.8 software (Camo Software, Norway) (Shaddad et al., 2016). PLSR models were validated using the 30% validation samples that were not included in the PLSR calibration stage. Models were then used to predict the six soil properties using the on-line collected soil spectra in September 2012 and 2014. The accuracy of these models are assessed by means of the ratio of prediction deviation (RPD), which equals the standard deviation of laboratory measured values divided by root mean square error of prediction (RMSEP). The following RPD classes proposed by Viscarra Rossel et al. (2006) were adopted in this study: RPD < 1.0 indicates very poor model predictions and their use is not recommended; an RPD between 1.0 and 1.4 indicates poor model predictions, where only high and low values are distinguishable; an RPD between 1.4 and 1.8 indicates fair model predictions, which may be used for assessment and correlation; an RPD between 1.8 and 2.0 indicates good model predictions, where quantitative predictions are possible; an RPD between 2.0 and 2.5 indicates very good quantitative model predictions; and an RPD > 2.5 indicates excellent model predictions.

2.3 Data processing

Data processing begun with kriging of the on-line VIS-NIR predicted soil properties and measured crop NDVI and yield. Kriged data layers were converted into a common 5 m^2 raster grid in ArcGIS (Esri, USA) to aid data fusion (Frogbrook and Oliver, 2007). The 5 m^2 raster grid was converted into a common grid of points that represented the value at the midpoint of each raster pixel. These steps ensured that all layers consisted of common sets of 5 m^2 grid points, essential for running the VNRX analysis. This method allowed fusion of data from a diverse range of soil and crop property (e.g., NDVI, Yield, etc.) surveys, measured at different resolutions (Khosla et al., 2008). However, it is worth noting that converting data from 5 m^2 raster squares to point locations introduced unavoidable errors to the data's spatial distribution. Finally, the different soil and crop layers of 5 m^2 grid were subjected to the VNRX non-linear parametric modelling, which is explained further in the following section.

2.4 Non-linear parametric modelling

The VNRX model, also known as nonlinear finite impulse response (NFIR) model, is used in this paper to represent a multi-inputs and single-output system. The model can be expressed as:

$$y(k) = f\left(u_1{}^{[k-1]}, u_2{}^{[k-1]}, \dots, u_R{}^{[k-1]}\right) + \varepsilon(k) \tag{1}$$

where $k(k = 1,2,..)$ is a time index, R is the number of system inputs, f is some unknown linear or non-linear mapping, which links the system output y to the system inputs $u_1, u_2, \dots, u_R$ and $\varepsilon(k)$ denotes the model residual. The symbol $u_i{}^{[k-1]}(i = 1,2, \dots, R)$ denotes the past information of the input u_i, which can be expanded as:

$$u_i{}^{[k-1]} = \bigcup_{j=0}^{n_i} u_i(k-j) \tag{2}$$

where n_i is the maximum temporal lag to be considered for the input u_i.

The Volterra series is a model for nonlinear behaviour that has similarities to the Taylor series. However, it differs from the Taylor series in its ability to capture 'memory' effects. The Taylor series can be used to approximate the response of a nonlinear system to given inputs if the output of this system depends strictly on the inputs at that particular time. In the Volterra series the output of the nonlinear system depends on the input to the system at all previous times. This provides the ability to capture the 'memory' effect of devices like capacitors and inductors (Tashev, 2009).

A commonly employed model type to specify the function f in Eq. (1) is a polynomial function (Chen and Billings, 1989; Wei et al., 2004), which can be expressed as:

$$y = \theta_0 + \sum_{m=1}^{N} \theta_m \emptyset_m + \varepsilon \quad (3)$$

where $\emptyset_m$ is the m^{th} model term generated from all input vectors, θ_m is the corresponding unknown parameters, and N is the total number of potential model terms. It is worth noting that $\emptyset_m$ is, in general, non-linear. Considering a system with two inputs u_1 and u_2, a second order polynomial function can be written as:

$$y = \theta_0 + \theta_1 u_1 + \theta_2 u_2 + \theta_3 {u_1}^2 + \theta_4 {u_2}^2 + \theta_5 u_1 u_2 + \varepsilon \quad (4)$$

The next step is to estimate the parameters $\theta_m (m = 0,1, \dots ,5)$ based on the observations $\{y, u_1, u_2\}$. The procedure begins by determining the structure, or the important model terms, using the orthogonal least squares (OLS) estimation procedures. It determines which dynamics and nonlinear terms should be included in the model by computing the contribution that each potential model term makes to the variation of the system output. The model is to be built up term by term in a manner that exposes the significance of each new term that is added. Once the structure of the model has been determined, the unknown parameters can be estimated, and the procedure of model validation can ensure the model is adequate. In this paper, a routine called adaptive-forward-orthogonal least squares (AFOLS) was employed, not only to determine the model structure, but also to estimate unknown parameters. The forward model selection scheme adopted consisted of a greedy optimisation algorithm that progressively includes additional terms into the model, starting from an empty structure, on the basis of the error reduction ratio (ERR) criterion (Cantelmo and Piroddi, 2010). It is a well-tested strategy for parsimonious modelling of data due to its effectiveness and merit to reduce ill conditioning and overfitting problems (Zhao et al., 2012).

The on-line measured soil properties (i.e., pH, MC, TN, P, K and TC) were normalised by removing the mean of each property, after which they were used as inputs to the VNRX model, whereas the model output was mean normalised crop yield and NDVI. The analysis also included the interaction between pairs of soil properties and their contribution to crop yield and NDVI. The aim was to investigate the contribution of each soil property and their pairwise interaction on crop NDVI and yield on one hand and to understand how the contribution varied amongst different cropping seasons on the other hand. To calculate the contribution of soil properties on yield, the NVRX analysis was carried out once in each cropping season in 2013 and 2015. However, for NDVI, the NVRX model was run twice per cropping season (e.g., May and June in 2013, and April and May in 2015). The VNRX modelling was carried out utilising Microsoft visual studio code written with C++ programming language.

Finally, the performance of the VNRX model in the prediction of NDVI and yield was evaluated by means of the of error reduction ratio (ERR) for each selected term calculated from AFOLS that measures the percentage this term contributes to the system output. Values of ERR always range between 0% and 100%. A higher ERR represents a greater dependence between this term and the output. Therefore, it is an important index for indicating the importance of each term to the output. To calculate the contribution of each input variable to the output, the sum of ERR values of all selected terms, denoted by $SERR$, and calculated by

$$SERR = \sum_{i=1}^{N}[err]_i \qquad (5)$$

was used to describe the percentage explained by the identified model to the system output, where N denotes the number of the selected terms. If the considered inputs can fully explain the variation of system output, the value of $SERR$ is equal to 100%. It is an indicator of model performance and uncertainty. The contribution of the i^{th} input variable to the variation of the system output, denoted as $ERRC_i$, is defined as the sum of ERR values of the terms that include this input variable. Because some selected terms may involve more than one input variable due to nonlinearity, the sum of $ERRC_i$ for all input variables can be greater than $SERR$. To overcome this problem, the value of $ERRC_i$ is used, which can be written as:

$$ERRC_i = \frac{\sum_{j=1}^{N}\left([err]_j | u_i \in \emptyset_j\right)}{\sum_{p=1}^{r}\sum_{j=1}^{N}\left([err]_j | u_p \in \emptyset_j\right)} \times SERR \quad (6)$$

The value of $ERRC_i$ should be always between 0% and 100%.

2.5 Mapping

Similar spatial distributions of measured versus predicted NDVI and yield were evaluated by comparing the corresponding maps. Maps were produced through interpolation with an inverse distance weighing (IDW) method, using ArcGIS software (ESRI, USA). The interpolation grid size of all maps had a radius of 12.5 m and a power of 2. The map cell size was 2.5 m^2 with 254 rows and 282 columns. Similarity between maps was assessed by visual comparison. In addition, Pearson's correlation (*r*) coefficient was calculated between each pair of data sets used to produce maps.

3. Results and discussion

3.1 Accuracy of on-line measured soil properties

The best independent validation of PLSR calibration models using on-line spectra (Table 1) is obtained for pH and TN with RPD values of 2.06 (very good prediction) and 1.85 (good model prediction), and RMSEP values of 0.434 and 0.013 (%), respectively (Shaddad, 2013). These results are better than those reported by Mouazen et al. (2007). Although both TC and MC have direct spectral responses in the NIR spectral range, they have not resulted in the best prediction accuracy in this study (Table 1). RPD values of P, TC and MC are rather small with values of 1.77, 1.50 and 1.49, respectively, which are classified as fair model predictions. The lowest RPD value of 1.31 is calculated for K, indicating poor prediction accuracy (Viscarra Rossel et al., 2006).

Table 1: Range of on-line measured soil pH, phosphorous (P), total nitrogen (TN), total carbon (TC), moisture content (MC) and exchangeable potassium (K) used in the Volterra Nonlinear Regressive with eXogenous inputs (VNRX) models.

Year	Range	pH	P (mg kg^{-1})	TN (%)	TC (%)	MC (%)	K (cmol kg^{-1})
2013	Min	5.31	20.33	0.11	1.46	11.98	0.18
	Max	7.83	56.21	0.18	2.40	17.41	0.31
2015	Min	5.87	26.83	0.05	0.92	4.53	0.22
	Max	6.44	43.34	0.16	1.81	9.79	0.47

3.2 Influences of soil properties on yield

Statistics for on-line measured soil properties used as input in the VNRX model are provided in Table 2. Observed ranges (e.g., minimum and maximum values) are different between 2013 and 2015, which can be attributed to farm practices (e.g., fertilisation) and different weather conditions affecting soil MC in particular.

Table 2: Validation of partial least squares regression (PLSR) models to predict soil pH, phosphorous (P), total nitrogen (TN), total carbon (TC), moisture content (MC) and exchangeable potassium (K) using on-line collected spectra of the prediction set.

	Soil properties					
Statistics	**pH**	**P (mg kg^{-1})**	**TN (%)**	**TC (%)**	**MC (%)**	**K (cmol kg^{-1})**
Sample no	48	23	22	24	45	24
Min	5.16	4.80	0.11	1.30	13.41	0.12
Max	8.17	50.00	0.20	2.46	24.28	0.40
Mean	6.46	22.50	0.15	1.79	18.03	0.23
SD	0.90	15.23	0.02	0.28	2.16	0.08
RMSEP*	0.43	8.61	0.01	0.18	1.45	0.06
R^2	0.73	0.69	0.72	0.57	0.56	0.44
RPD	2.06	1.77	1.85	1.50	1.49	1.31
Model quality**	A	B	A	B	B	C

*RMSEP: Root mean square error of prediction; **Model quality is categorized according to Viscarra Rossel et al. (2006) (A: residual prediction deviation (RPD)>1.8; B: RPD=1.4–1.8; C: RPD<1.4).

Based on Eq. (3), the polynomial model to express the relationship between the six input soil variables and the output NDVI and yield is of quadratic terms, written as:

$$y = \theta_0 + \sum_{i=1}^{6} \theta_i u_i + \sum_{i=1}^{6} \sum_{j=i}^{6} \theta_{ij} u_i u_j + \varepsilon \qquad (7)$$

This model includes 28 terms consisting of 7 linear terms $\{\theta_{0,}\ \theta_i u_i | i = 1,2,\ldots,6\}$ and 21 nonlinear terms $\{\theta_{ij} u_i u_j | i = 1,2,\ldots,6; j = i, i+1,\ldots,6\}$. The main reason for selecting quadratic instead of cubic terms is to balance the number of candidate terms and number of samples. If cubic terms are considered, there are 84 candidate terms, which require a large memory and high computational cost to implement the algorithm based on 7187 sampled points. A model with cubic terms was tested and revealed no significant differences in results, hence, the quadratic terms' model was adopted.

Values of ERRC calculated by Eq. (6), explaining the contribution of individual soil properties to the crop yield in 2013 and 2015 cropping seasons, are shown in Table 3. To evaluate the change of model uncertainty, the value of $SERR$ needs to be examined. It is observed that the $SERR$ value in 2013 (21%) was larger than the corresponding value in 2015 (12.51%), which could be attributed to varying weather conditions that exert a big impact on crop growth and yield (Renouf et al., 2010; Boone et al., 2016), or to errors in the estimation models (both kriging and PLSR models). Other affecting factors that vary through cropping seasons are pests, which are similarly associated with different weather conditions, but are strongly linked to crop variety (Eberhart and Russell, 1966; Paveley et al., 2012). Finally, the different crops grown throughout the experiment (in 2013 and 2015) represents one of the major factors that explaining why contribution of soil properties to yield differ through the two cropping seasons.

Table 3: Calculated individual contribution (ERRC) of normalised on-line soil properties on wheat and spring barley yields in 2013 and 2015, respectively.

	ERRC	
Input	**2013**	**2015**
K (cmol kg^{-1})	7.66	0.23
P (mg kg^{-1})	4.28	1.96
TC (%)	3.99	3.23
pH	3.51	1.45
TN (%)	1.56	4.46
MC (%)	0.00	1.18
Total (SERR)	21.00	12.51

TC is total carbon, TN is total nitrogen, K is exchangeable potassium, P is extractable phosphorous and MC is moisture content.

Observations show that K, P and TC contribute most to wheat yield in 2013, whereas TC and TN contribute most to spring barley yield in 2015. The largest contributor to wheat yield in 2013 is K ($ERRC$ = 7.66%) followed by P, which represent key nutrients to crop growth and development (Baligar et al., 2001). This is the reason why P and K together with nitrogen are applied annually. However, this is not the case for the spring barley in 2015, at least for K. It seems that TC retains almost the same contribution to wheat yield in 2013 and spring barley yield in 2015, which may be explained by nutrient demands varying between crops. For example, wheat requires about 200 kg N, 55 kg P2O5 and 252 kg K2O/ha (Roy et al., 2006), whereas the UK national averages are 175 kg, 69 kg and 212 kg ha^{-1}, respectively. Furthermore, nutrient requirements for the same crop vary between seasons and have to be checked every 3 to 5 years (Nicholls, 2015). Depending on the cropping system, carbon in the form of organic fertilisers is frequently added to agriculture fields, as it supports photosynthesis (Ravikumar, 2013) and improves soil structure and hydraulic conductivity. Therefore, it is unsurprising to observe that TC is a strong contributor to yield in both study years. pH was a persistently strong contributing soil property, particularly in 2013. An acidic or basic soil can prevent nutrient uptake and thus impede plant production (Schubert et al., 1990). Farmer's guides commonly argue that the optimum pH for soils under continuous arable cropping (wheat and barley) is between 6 and 7 with 6.5 being optimum. Since the soil pH range in this study is wider than the optimum range (Table 2), pH is considered to have an influence on nutrient availability and subsequently yield. Although TN contribution ranks 5^{th} in 2013, it has the largest contribution to yield in 2015. The narrow variation range over two sampled years: 2013 (0.05 to 0.16%), and 2015 (0.11 to 0.18%) (Table 2) may explain the fluctuated $ERRC$ value of TN to yield (Table 3). MC has low yield contribution, where the $ERRC$ value in 2013 is null. This could be explained by the time difference between MC and yield measurements. However, this time difference has only a minor influence on the remaining five soil properties considered in this study, as they are much less dynamic compared to MC.

3.2 Influences of soil properties on NDVI

Table 4 shows calculated $ERRC$ and $SERR$ values for NDVI in 2013 and 2015 based on the on-line measured soil properties in 2013 and 2015, respectively. $SERR$ values, indicating the total contribution of soil properties to NDVI (Table 4), are much larger than the corresponding figures for yield (Table 3). These are 30.92% and 35.42% for May and June 2013, and 48.59% and 11.35% for April and May 2015, respectively. However, $SERR$ value in May 2015 is notably low (11.35%), which can be attributed to a drought period occurring mid growing season; where the combination of a dry March and the sunniest April on record with little rainfall was recorded (UK Meteorological Office). This is because NDVI measurement took place at the booting growing stage, at which point the crop is particularly susceptible to drought and certain diseases. Elsewhere, a decrease in growth rate has been attributed to drought imposed at various growth stages in wheat, among which booting was listed (Ashraf, 1998).

Table 4: Calculated individual contribution (ERRC) of normalised on-line measured soil property to normalised difference vegetation index (NDVI) of wheat and spring barley in 2013 and 2015, respectively.

	ERRC			
	2013		**2015**	
Input	**May**	**June**	**April**	**May**
TC (%)	10.25	16.46	5.86	3.52
K (cmol kg^{-1})	9.82	3.19	5.90	4.12
P (mg kg^{-1})	6.00	12.33	31.31	0.00
pH	2.69	0.91	3.21	0.00
MC (%)	1.71	1.39	2.31	2.83
TN (%)	0.45	1.14	0.23	0.88
Total (SERR)	30.92	35.42	48.59	11.35

TC is total carbon, TN is total nitrogen, K is exchangeable potassium, P is extractable phosphorous and MC is moisture content.

Similar to crop yield (Table 3), K ($ERRC$ = 9.82% and 3.19%) and P ($ERRC$ = 6% and 12.33%) are the largest contributors to NDVI after TC ($ERRC$ = 10.25% and 16.46%) in 2013 (Table 4). A similar trend can be observed for NDVI response in 2015, where K, P and TC are again the largest contributors to NDVI (Table 4), except P in May. It is important to note that P contribution to NDVI surges in April 2015, with a $ERRC$ value of about 6 times of those of K and TC. Phosphorus is an essential nutrient for both plant structural compounds and energy conversion (Ozanne et al., 1980). P availability is essential for crop growth during spring. For example, Grant et al. (2001) reported for a barley crop that during the period from March to May, 70% of phosphate is taken up. This may explain the surge in P contribution to NDVI in the April 2015 measurement. pH, MC and TN have low contributions to NDVI in both years.

3.3 Prediction of NDVI and yield based on on-line measured soil properties

To evaluate the performance of the proposed model for predicting NDVI and yield based on on-line measured soil properties, the first five terms ranked by $ERRC$ were selected, and the corresponding parameters were estimated, to establish the following model:

$$y = \theta_0 + \sum_{m=1}^{5} \theta_m \emptyset_m \quad (8)$$

The input variables used are the normalisation values obtained with mean normalisation. Table 5 shows the first five (largest contributors) individual and interaction terms to describe the relationship between on-line measured soil properties and NDVI and yield in 2013 and 2015 cropping seasons. Generally, TC, P, K and MC are the most influential variables on NDVI in the two experimental years. Among the interaction terms, TC * K appears first in June 2013 and April 2015 measurements, whereas MC * TC appears first in May 2013 and 2015. Interaction P * K is the second most contributing term to NDVI in June, 2013. Once again this confirms the high individual and interaction contributions of TC, P and K on crop NDVI for the two studied cereal crops.

Examining interaction effects of soil properties on yield reveals almost a similar trend to that of NDVI, where K, P and TC are the most influential individual factors in 2013 only, whereas no individual influence for K and P can be observed in 2015 (Table 5). However, MC is not part of the most influential interactive terms anymore, and is instead replaced by pH. This may be attributed to the drought impact during spring in 2015, according to the UK Meteorological Office. Both pH * K and TN * P are the most influential interaction terms on yield in 2013, whereas TN * K and pH * P are the most important interaction terms in 2015. Although N, P and K are key nutrients for crop growth and yield, pH is important for nutrient availability to plants (Schubert et al., 1990).

NDVI and yield can now be predicted, by substituting values of on-line measured soil properties into Eq. (8) using coefficients shown in Table 5. A map showing the spatial distribution of predicted versus measured NDVI and yield is shown in Fig. 3 and Fig. 4, respectively.

Table 5: Individual and interaction relationship between on-line measured soil properties and normalised difference vegetation index (NDVI) and yield for data collected in 2013 and 2015. The order of the terms was ranked by the calculated individual contribution (ERRC) of each soil property.

	Month		**0**	**1**	**2**	**3**	**4**	**5**
NDVI	**May-13**	$\emptyset_m$*	constant	**P**	**TC**	**K**	**K^2**	**TN*MC**
		θ_m**	0.45	-0.003	0.095	0.7	16.45	0.804
	Jun-13	$\emptyset_m$	constant	**TC**	**P**	**TC*K**	**P*K**	**pH*K**
		θ_m	0.488	0.1	-0.002	2.159	-0.036	-0.397
	Apr-15	$\emptyset_m$	constant	**P**	**K*TC**	**MC**	**pH**	**TC**
		θ_m	0.345	0.014	3.798	0.024	-0.162	-0.068
	May-15	$\emptyset_m$	constant	**K**	**TC**	**MC**	**MC*TC**	**TN^2**
		θ_m	0.485	0.297	-0.069	0.006	-0.032	13.589
Yield	**2013**	$\emptyset_m$	constant	**K**	**pH*K**	**TN*P**	**P**	**TC**
		θ_m	6.711	13.712	-21.677	1.902	-0.036	1.226
	2015	$\emptyset_m$	constant	**TN**	**TC**	**TN*K**	**pH^2**	**pH*P**
		θ_m	8.449	35.843	-2.457	-153.7	6.971	-0.279

*$\emptyset_m$: Model term; **θ_m: coefficient of the model term

Observations show that similarities exist between the spatial distributions between each pair of maps, particularly for NDVI. Interestingly, there is a distinct similarity between NDVI and yield maps in 2013 (high *r* values in Table 6) for both measured and predicted maps (Figs. 3 and 4). Conversely, similarities in 2015 for both measured and predicted maps are not clear (low r values in Table 6). The poor similarities shown in the 2015 cropping season may be attributed to deterioration in PLSR prediction accuracy for the on-line collected soil data in 2015, since PLSR calibration models were developed on the basis of samples collected in 2013. This could also explain the drop in the total contribution of soil properties to yield (SERR = 12.51) and low *r* (Table 6). Another potential explanation is that external factors not accounted for in this study (e.g., fungi diseases) have a stronger influence on crop yield in 2015 than in 2013.

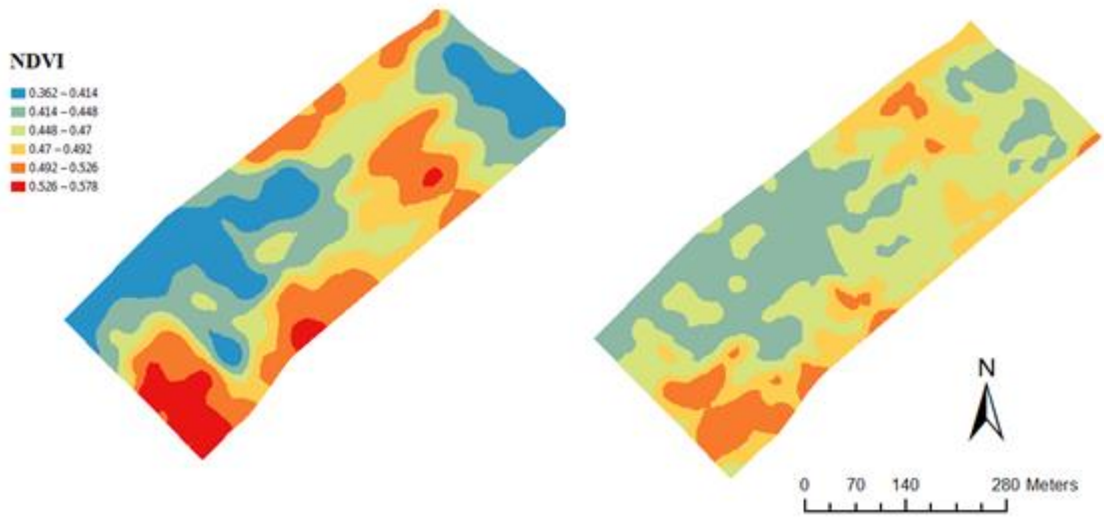
Pearson correlation coefficient values shown in Table 6 demonstrate that the prediction performance for NDVI is more successful than yield in three out of four occasions. This observation is supported by the fact that SERR values for NDVI are consistently higher than the corresponding values for yield (Tables 3 and 4). The highest SERR value of 48.59% is calculated for NDVI prediction in April 2015 (Table 4), which is in line with the highest *r* value of 0.71 calculated between measured and predicted values (Table 6).

Table 6: Pearson correlation coefficient (*r*) values between measured and predicted crop yield and normalised difference vegetation index (NDVI), based on Eq. (8) and identified terms and coefficients shown in Table 5. The crops were wheat and spring barley in 2013 and 2015, respectively.

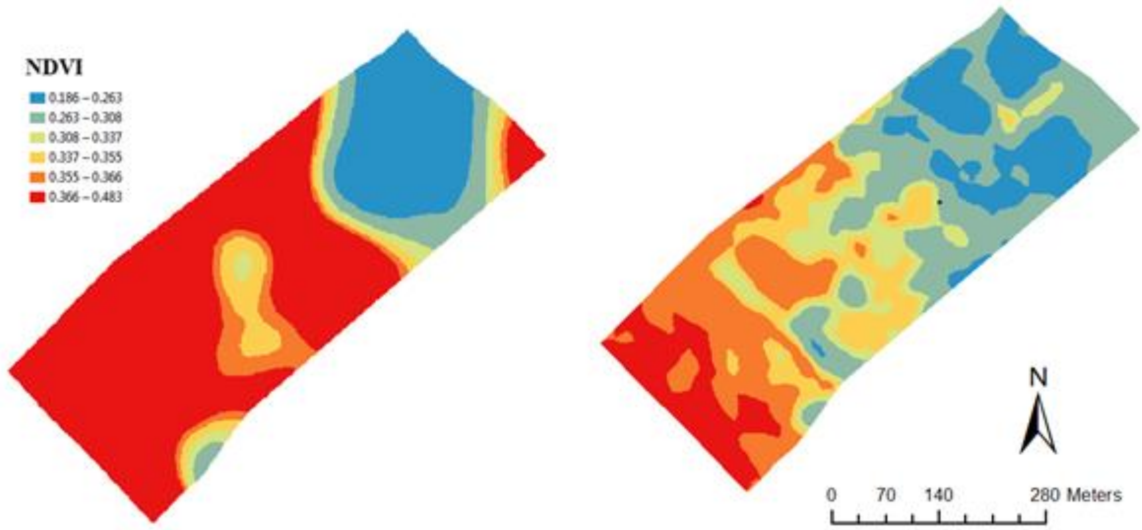
Year	Output	Correlation coefficient
2013	Yield	0.48
2015	Yield	0.38
2013	NDVI May	**0.56**
2013	NDVI June	**0.60**
2015	NDVI April	**0.71**
2015	NDVI May	0.40
2013	NDVIm (May) vs Yieldm	**0.60**
2013	NDVIp (May) vs Yieldm	**0.40**
2013	NDVIp (May) vs Yieldp	**0.83**
2015	NDVIm (April) vs Yieldm	0.12
2015	NDVIp (April) vs Yieldm	0.10
2015	NDVIp (April) vs Yieldp	0.25

The significance threshold is 0.062 at 95% confidence level, NDVIm is measured NDVI, NDVIp is predicted NDVI, Yieldm is measured yield and Yieldp is predicted yield

Although *r* values are larger for NDVI than for yield during the two cropping seasons (Table 6), it is not recommended to rely on only the six on-line measured soil properties to predict yield. Low *r* values for yield could be attributed to the exclusion of other factors affecting yield and encountered at late growing stages such as soil compaction, inter plant competition, fungal disease and insect pressures (Donald, 1963; Cannell et al., 1980; Coakley, 1988; Paveley et al., 2012). The latter factors have high spatial variability and can reduce yields by up to 7 tonne ha^{-1} (Bravo et al., 2003). Therefore, it is suggested to expand the current work by accounting for other soil properties and diseases, alongside weather conditions, which is considered the most influential factor controlling the distribution and severity of fungal infections (Dammer, 2006).



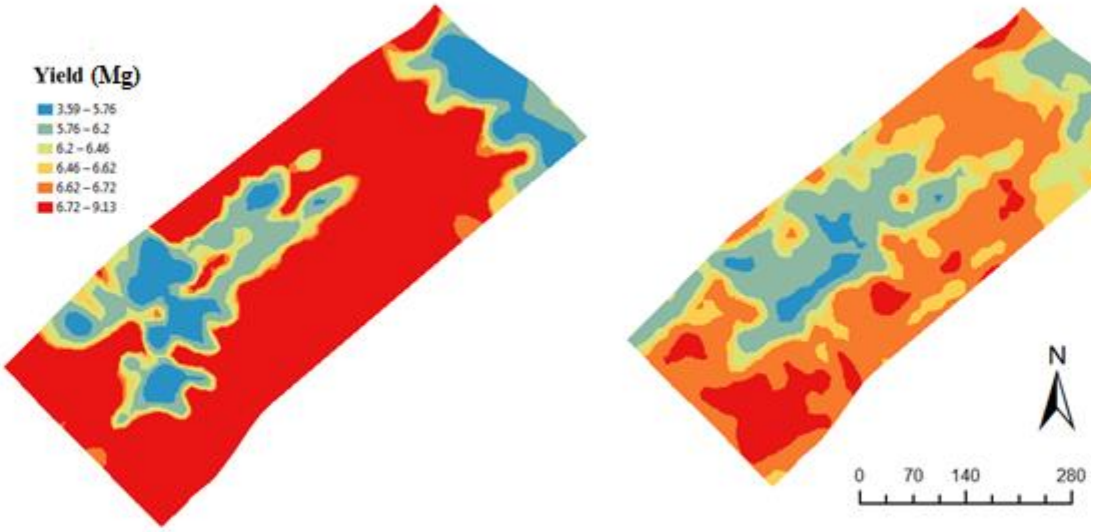
(a)



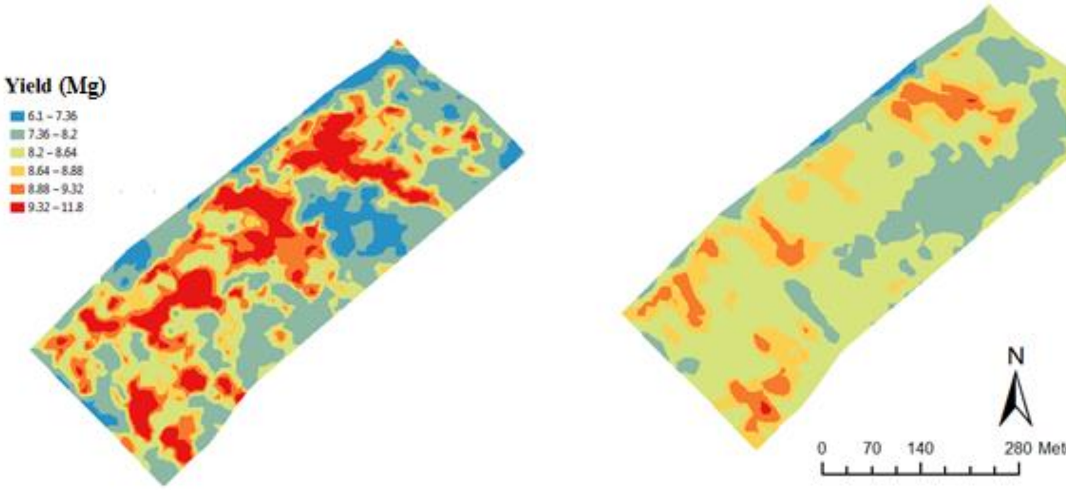
(b)

Fig. 3. Comparison between measured (right) and predicted (left) normalised difference vegetation index (NDVI) based on Eq. (8) and corresponding terms and coefficients shown in Table 5 for May 2013 (a) and April 2015 (b).

This study has presented a novel application of nonlinear parametric modelling technique based on a Volterra Nonlinear Regressive with eXogenous inputs (VNRX) model to study the influences of six soil properties: total nitrogen (TN), total carbon (TC), moisture content (MC), potassium (K), phosphorous (P) and pH. Soil properties were collected at high



(a)



(b)

Fig. 4. Comparison between measured (right) and predicted (left) crop yield using the model of Eq. (8) and corresponding terms and coefficients shown in Table 5 for wheat in 2013 (a), and spring barley in 2015 (b).

sampling resolution with an on-line soil sensor on crop yield and normalised difference vegetation Index (NDVI). The analysis was carried out in two cropping seasons in 2013 (wheat) and 2015 (spring barley). The results provided for the following conclusions:

1. The performance of the VNRX model in the prediction of yield evaluated with the error reduction ratio contribution (ERRC) indicated that different soil properties have different influences on yield. K, P and TC were the highest contributors to wheat yield and TN, TC and P to spring barley.
2. Sum of error reduction ratio (SERR) showed soil property contributions to NDVI to be higher than those to yield, with TC, K and P being the most influencing factors. The highest SERR value of 48.59% was calculated for NDVI, which was in line with the highest Pearson correlation coefficient (*r*) of 0.71 calculated between measured and predicted NDVI.
3. The highest influential interaction terms of soil properties on NDVI were TC * K, and MC * TC, whereas the most important terms for yield were pH * K and TN * P for wheat and TC * K and pH * P for spring barley. These contributions may vary among different fields, crops, weather conditions and soil fertility status.
4. Although VNRX models allowed the prediction of yield and NDVI to a given degree of success, relatively low correlations between measured and predicted yield necessitate a need to understand other influencing factors (i.e., weather conditions, disease and other soil properties), to improve VNRX model predictions.

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Nonlinear parametric modelling to study how soil properties affect crop yields and NDVI

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