



DE EXTREMADURA





DEPARTAMENTO DE EXPRESIÓN GRÁFICA

TESIS DOCTORAL

MINERÍA DE DATOS EN EL ANÁLISIS DE LAS FIRMAS DE CULTIVOS AGRÍCOLAS

PHD THESIS

DATA MINING IN THE ANALYSIS OF CROP SIGNATURES

FERNANDO RODRÍGUEZ MORENO

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CONFORMIDAD DEL DIRECTOR FDO: ÁNGEL MANUEL FELICÍSIMO PÉREZ

El doctor Don <i>Ángel Manuel Felicísimo Pérez</i> informa que:					
La memoria titulada Minería de datos en el análisis de las firmas de cultivos agrícolas , que presenta Fernando Rodríguez Moreno, Licenciado en Ciencias Ambientales, para optar al grade de Doctor, ha sido realizada en el Departamento de Expresión Gráfica de la Universidad de Extremadura, bajo mi dirección y reuniendo todas las condiciones exigidas a los trabajos de tesis doctoral.					
	Badajoz, Febrero de 2013.				
Fdo.: Ángel Manuel Felicísimo Pérez					

"The scientist is free, and must be free to ask any question, to doubt any assertion, to seek for any evidence, to correct any errors." J. Robert Oppenheimer

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A mis padres, a mi director de tesis, a mi... no es fácil escribir este apartado siendo justo porque el camino ha sido largo y duro.

En ocasiones la ayuda era premeditada, en otras resultó fruto del azar, a veces surgió en el momento y lugar menos esperado, otras fue fruto de algún desencuentro.

Esta tesis es el resultado de una estupenda partida de billar. Hoy contemplo satisfecho el buen trabajo y quiero darle las gracias a todos aquellos que me dedicaron tiempo porque todos ellos participaron en esa partida de billar, todos ellos me han traído aquí, por eso, muchas gracias.

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To my parents, my supervisor, my ... not easy to write this section being fair because the road has been long and hard.

Sometimes the help was premeditated, in other was haphazard, sometimes emerged when and where least expected, others were the result of a misunderstanding.

This thesis is the result of a great game of pool. Today I look satisfied the good work and I want to thank everyone who spent time with me because they all participated in the game of pool, all of them have brought me here, so, thank you very much.

A mis padres 🥴

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Introducción / Introduction

Necesidades del agricultor / Farmers' needs

Los agricultores son cada día más conscientes de la necesidad de aplicar el tratamiento agronómico específico que precisa el cultivo de tal forma que el rendimiento de los insumos sea máximo y el desarrollo sostenible (Barker and Pilbeam 2007; Jones 1998; Marschner 1995; Mengel and Kirkby 2001). De esta forma se obtiene el máximo beneficio hoy y se garantiza la rentabilidad de la actividad agrícola en el futuro.

En la consecución de esta meta la agricultura de precisión juega un papel determinante. La agricultura de precisión pone a disposición del agricultor la última tecnología (Srinivasan 2006; Stafford 1997), gracias a la cual es posible cartografiar de forma precisa, rápida y barata el campo y aplicar un tratamiento diferencial ajustado a las necesidades específicas de cada una de las unidades tierra que lo componen.

La correcta delimitación de las unidades tierra así como el certero diagnóstico agronómico de las mismas se puede conseguir aunando conocimientos agronómicos y técnicas de minería de datos, evidenciarlo es el propósito de esta tesis. Este binomio está fuera del alcance de muchos agricultores por lo que es necesario desarrollar metodologías de muestreo/análisis más sencillas y tratar de desarrollar sistemas de apoyo a la decisión, de forma que el agricultor pueda encontrar las respuestas que necesita con la ayuda de su consultor agrícola y del laboratorio.

Farmers are increasingly aware of the need for specific agronomic treatment, the required for the crop such that the input performance is maximized and the development is sustainable (Barker and Pilbeam 2007; Jones 1998; Marschner 1995; Mengel and Kirkby 2001). Thus the farmer gets the maximum benefit today and ensures the profitability of the farm in the future.

Precision agriculture plays a key role in achieving that goal. Precision agriculture offers to the farmer the latest technology (Srinivasan 2006; Stafford 1997), thanks to which it is possible to map accurately, quickly and cheaply the field and apply differential treatment adjusted to the specific needs of each of the land units

Proper delineation of land units and its correct agronomic diagnosis can be obtained by combining agricultural knowledge and data mining, the purpose of this thesis is to prove it. This binomial is beyond the reach of many farmers so it is necessary to develop methodologies for a simple sampling / analysis and try to develop a decision support system, so the farmer can find the answers with the help of his agricultural consultant and laboratory.

Soluciones actuales / Current solutions

Gracias a numerosos estudios agronómicos se han conseguido identificar los rangos de concentraciones y las relaciones entre las concentraciones de los nutrientes adecuadas para la mayoría de los cultivos (Marschner 1995; Rengel 1998; Reuter *et al.* 1998). Rangos de suficiencia y relaciones que pueden emplearse como referencia en la elaboración de los planes de fertilización, de esta forma es más probable que el agricultor alcance altos y sostenibles rendimientos del cultivo.

El procedimiento tradicional para la obtención de las concentraciones de los nutrientes en la planta son los análisis foliares. Su obtención requiere trabajo de campo (muestreo) y de laboratorio (análisis), es por tanto costosa en tiempo y recursos. Si es necesaria una estimación rápida y barata, entonces la solución son las medidas de la reflectancia espectral del cultivo (medidas proximales o remotas). Son muchos los trabajos científicos que han demostrado el potencial de la radiometría para estimar la concentración de los diferentes nutrientes en la planta (Bannari *et al.* 2007; Cammarano *et al.* 2011; De Assis Carvalho Pinto *et al.* 2007; Gnyp *et al.* 2009; Goel *et al.* 2003; Gómez-Casero *et al.* 2007).

Hoy existen numerosos dispositivos comerciales (Abdelhamid *et al.* 2003; Arregui *et al.* 2006; Castelli and Contillo 2009; Graeff *et al.* 2009), muchos de ellos sencillos dispositivos de mano programados con intuitivas interfaces de usuario, que ofrecen estimaciones del nivel de los nutrientes en la planta obtenidas a partir de las lecturas que el agricultor puede obtener en unos pocos minutos de muestreo en campo.

It has been possible to identify the ranges of concentrations and relations between the concentrations of nutrients suitable for most crops thanks to numerous agronomic studies (Marschner 1995; Rengel 1998; Reuter *et al.* 1998). Sufficiency ranges and relationships that can be used as a reference to calculate the fertilization plan, so it is more likely that farmers achieve high and sustainable crop yields.

The traditional procedure for obtaining the concentrations of nutrients in the plant is leaf analysis. Its obtaining requires fieldwork (sampling) and laboratory (analysis), it is therefore costly in time and resources. Whether a rapid and inexpensive estimation is necessary, then the solution is spectral reflectance measurements of the crop (proximal or remote measurements). Many scientific studies have shown the potential of radiometry to estimate the concentration of different nutrients in the plant (Bannari *et al.* 2007; Cammarano *et al.* 2011; De Assis Carvalho Pinto *et al.* 2007; Gnyp *et al.* 2009; Goel *et al.* 2003; Gómez-Casero *et al.* 2007).

Today there are numerous commercial devices (Abdelhamid *et al.* 2003; Arregui *et al.* 2006; Castelli and Contillo 2009; Graeff *et al.* 2009), many of them simple handheld devices programmed with intuitive user interfaces, which provide estimates of the level of nutrients in the plant derived from the readings that the farmer can get in a few minutes of field sampling.

Problemas actuales / Current problems

Los anteriormente comentados rangos de suficiencia para las concentraciones de los nutrientes son específicos del cultivo e incluso del cultivar, además requieren el muestreo de una parte determinada de la planta en un estado fenológico concreto (Marschner 1995; Rengel 1998). Otro problema de los rangos de suficiencia es que sólo han sido validados en unas determinadas condiciones, las de los ensayos en las que fueron determinados, las cuales no pueden abarcar todas las combinaciones posibles de desarrollo del cultivo (Alves Mourão Filho 2005; Camacho *et al.* 2012; Jeong *et al.* 2009; Stalenga 2007). El caso de las metodologías que emplean relaciones entre nutrientes es diferente, son más generalizables en el espacio y tiempo, aunque las limitaciones anteriores no ha desaparecido (Agbangba *et al.* 2011; Amundson and Koehler 1987; Dagbénonbakin *et al.* 2010).

Las firmas espectrales del cultivo, procedentes de medidas proximales o remotas, se transforman en estimaciones de los niveles de los nutrientes en la planta mediante modelos que poseen una baja capacidad de generalización espacio-temporal. Esto reduce su efectividad en explotaciones agrícolas reales (Heege *et al.* 2008; Li *et al.* 2010), relegando al binomio agronomía-radiometría a los grandes campos dónde resulta imbatible en la actualidad. En esos escenarios una pequeña mejora por unidad de superficie supone un gran incremento en los beneficios, es por ello que hasta pueden llegar a disponer de un panel de expertos que realicen estudios de calibración.

Si no mejora la efectividad y capacidad de generalización de los modelos que relacionan las firmas espectrales (reflectancia) del cultivo y las concentraciones de nutrientes en la planta, el aumento del rendimiento del cultivo y de la sostenibilidad posibles gracias a la agricultura de precisión (radiometría), no llegará a todas las explotaciones agrícolas.

The previously mentioned sufficiency ranges for concentrations of nutrients are crop specific and even of the cultivar. It also requires the sampling of a particular part of the plant in a particular phenological stage (Marschner 1995; Rengel 1998). Another problem, the sufficiency ranges have been validated in certain conditions, the conditions of the trials in which they were determined, which cannot cover all possible combinations of crop development (Alves Mourão Filho 2005; Camacho *et al.* 2012; Jeong *et al.* 2009; Stalenga 2007). The case of the methodologies use relationships between nutrients is different; it is more generalizable over space and time, although the above limitations are not gone (Agbangba *et al.* 2011; Amundson and Koehler 1987; Dagbénonbakin *et al.* 2010).

The crop spectral signatures, from proximal or remote measures, are transformed into estimates of the levels of nutrients in the plant using models that have low space-time generalization ability. This reduces its effectiveness in real farms (Heege *et al.* 2008; Li *et al.* 2010), relegating the binomial agronomy-radiometry to large areas where it is currently unbeatable. In these scenarios a small improvement per unit area is a large increase in profits, which is why they may even have a panel of experts to carry out calibration studies.

If the effectiveness and generalizability of the models do not improve, the increase in crop yield and sustainability possible thanks to precision agriculture will not reach all farms.

Propósito de esta tesis / Purpose of this thesis

El propósito de esta tesis es realizar dos aportaciones significativas en el campo de la agricultura de precisión. Ambas aportaciones persiguen el mismo objetivo, aumentar la eficacia y reducir los costes de los diagnósticos agronómicos integrales. En caso de conseguirlo aumentaría el número de explotaciones agrícolas que pueden apostar por la agricultura de precisión. Esa resultaría ser la opción más rentable tanto para el presente como para el futuro.

Una explicación simplificada del proceso de diagnóstico agronómico sería adquisición de información relevante del cultivo e interpretación de la misma, los dos procesos a los que esta tesis dirige la atención. Se pretende mejorar la efectividad y capacidad de generalización de los modelos que estiman el estado nutricional de la planta a partir de medidas espectrales. También se trata de incorporar las técnicas geomáticas desarrolladas en las últimas décadas (GPS, GIS,...) a las metodologías clásicas para la interpretación de los niveles de los nutrientes en la planta. El objetivo es desarrollar una metodología para el diagnóstico agronómico de los campos, sería un proceso lógico deductivo que trabaja con evidencias obtenidas en el mismo campo. No serían precisos estudios previos y por tanto estaría a disposición de cualquier agricultor independientemente del área geográfica o cultivo.

The purpose of this thesis is to make two significant contributions in the field of precision agriculture. Both contributions have the same objective, to increase efficiency and reduce the costs of comprehensive agronomic diagnosis. In case of achieving the objectives, this would increase the number of farms that can go for precision agriculture. It would be the most profitable option for the present and the future.

A simplified explanation of the process for the agronomic diagnostic would be the acquisition of relevant information of the crop and interpretation of the same, the two processes to which this thesis directs the attention. It is intended to improve the effectiveness and generalizability of models that estimate the nutritional status of the plant from spectral measurements. On the other hand tries to incorporate the techniques developed in the last decades (GPS, GIS ...) to the classical methods for the interpretation of the levels of nutrients in the plant. The purpose is to develop a methodology to make agronomic diagnosis; it would be a deductive process that works with evidence obtained in the same field. No previous studies would be needed and therefore it would be available to all farmers, regardless of geographic area or crop.

Estructura y contenido de la tesis / Structure and content of the thesis

Índices espectrales de vegetación / Spectral vegetation indices

La tesis comienza evaluando el verdadero potencial de los 21 índices espectrales de vegetación (radiometría) más ampliamente usados para estimar la concentración de un nutriente, el nitrógeno, en planta (Blackburn 2007; Panda *et al.* 2010; Raymond Hunt *et al.* 2011; Schellberg *et al.* 2008). Prueba realizada en unas condiciones que simulan una explotación agrícola real (amplio rango de condiciones de desarrollo). Es preciso conocer si los índices espectrales de vegetación son una solución en la práctica, si empleándolos es posible obtener estimaciones correctas, rápidas y baratas del estado nutricional del cultivo. En caso afirmativo habría que dirigir los esfuerzos a proyectos de demostración con los que animar la transferencia de la tecnología a los agricultores.

The thesis begins by evaluating the true potential of 21 spectral vegetation indices (radiometry), the most widely used indices to estimate the concentration of a nutrient, the nitrogen, in plant (Blackburn 2007; Panda *et al.* 2010; Raymond Hunt *et al.* 2011; Schellberg *et al.* 2008). Testing conducted under conditions that simulate real farms (wide range of growing conditions). It is necessary to know if spectral vegetation indices are a practical solution, if it is possible to obtain correct, fast and cheap estimates of the crop nutritional status. If so efforts should be directed to demonstration projects which encourage the transfer of technology to the farmers.

Garantías exigidas en el estudio / Guarantees required in the study

En esta tesis se dedica un apartado especial al procedimiento de evaluación de los resultados. Confundir una relación descriptiva con una predictiva conduciría al desarrollo de un modelo cuyas recomendaciones no tendrían ningún valor, lo que haría que los objetivos de la tesis fueran inalcanzables. Para obtener evaluaciones realistas se toman 4 medidas, una ya comentada, experimentar en un amplio rango de condiciones de desarrollo. La segunda medida consiste en forzar al modelo que ha de relacionar el índice espectral de vegetación y la concentración de nutriente a que sea válido durante todo el período durante el cual sería posible actuar para corregir una potencial deficiencia (novedad). La tercera medida es el uso de la validación cruzada en la evaluación de las relaciones y la cuarta medida es el empleo en el ensayo del cultivo que presenta mayores dificultades para el desarrollo de modelos radiométricos, el triticale de doble propósito.

Verato es el cultivar del triticale (X *Triticosecale* Wittmack) que soporta el pastoreo del ganado durante su desarrollo sin arruinar la cosecha final. Esta peculiaridad dificulta la consecución del objetivo, el desarrollo de un modelo radiométrico eficaz y generalizable, al no poder confiar en el verdor como estimador de la concentración de nitrógeno (después del pastoreo el cultivo amarillea debido a un desajuste entre crecimiento y síntesis de clorofila, no por déficit de nitrógeno). Eso obliga a

la búsqueda de rasgos espectrales más directamente relacionados con la concentración de nitrógeno, los cuales respondan correctamente incluso en condiciones complicadas.

Gracias a estas medidas se pretende determinar el umbral mínimo de eficacia de la metodología, se aumentan las garantías de poder predictivo del modelo y se reducen costes de implementación, facilitando así la transferencia de los resultados a explotaciones agrícolas reales.

This thesis has a special section to describe the procedure of evaluating the results. Mistaking a descriptive relationship with a predictive relationship leads to the development of a model whose recommendations would have no value; in that case the objectives of the thesis would be unreachable. For realistic assessments four measures were taken, the first has already been mentioned, experimentation in wide range of growing conditions. The second measure consists in forcing the model (the model that has to relate spectral vegetation index and nutrient concentration) to be valid in the period during which one could act to correct a potential shortcoming (new). The third measure is the use of cross-validation in the evaluation of relationships and the fourth measure is employment in the test of a crop that presents superior difficulties for the development of radiometric models, the dual purpose triticale.

Verato is the cultivar of triticale (X *Triticosecale* Wittmack) that supports livestock grazing during its development without ruining the final harvest. This peculiarity makes difficult to achieve the objective, the development of an effective and generalizable radiometric model, because with that crop the green of the plant is not a good estimator of the nitrogen concentration (after grazing the crop yellowing due to a mismatch between growth and chlorophyll synthesis, no nitrogen deficiency). That requires finding spectral features directly related to the concentration of nitrogen, which respond correctly even in difficult conditions.

Thanks to these measures the minimum threshold of effectiveness of the methodology could be determined; they increase the guarantees of predictive power and reduce implementation costs, thus facilitating the transfer of results to the real farms.

Técnicas de reducción de dimensiones / Techniques for dimensionality reduction

En el mismo escenario y con los mismos datos y procedimiento de evaluación se estudia si las dos técnicas de reducción de dimensiones más potentes, Análisis de componentes principales (PCA) (Shlens 2005) y Análisis de componentes independientes (ICA) (Hyvärinen and Oja 2000), son adecuadas para el procesamiento de los datos obtenidos en el muestreo hiperespectral del cultivo (firma espectral completa). Si las técnicas son efectivas entonces concentrarán la información relativa al estado nutricional del cultivo en una decena de nuevas componentes, con las que sería fácil desarrollar modelos de regresión con los que estimar eficazmente la concentración de nitrógeno en planta.

Un resultado positivo en el estudio con las técnicas de reducción de dimensiones difícilmente sería un resultado transferible, esto es así dado el coste del espectroradiómetro necesario para obtener la firma espectral. El objetivo de este estudio es dar un paso intermedio, comprobar que aún con todas las

garantías exigidas es posible desarrollar un modelo efectivo con capacidad de generalización en el espacio y tiempo (dentro de la misma campaña).

In the same scenario and with the same data and evaluation procedure, it was studied whether the two techniques for dimensionality reduction more powerful, Principal component analysis (PCA) (Shlens 2005) and Independent Component Analysis (ICA) (Hyvärinen and Oja 2000), are suitable for processing the data obtained in the hyperspectral sampling of the crop (spectral signature). If the techniques are effective then they will concentrate the information about the nutritional status of the crop in a dozen new components, with which it would be easy to develop regression models to effectively estimate the nitrogen concentration.

A positive result in the study with the techniques for dimensionality reduction would hardly be a transferable result; this is because the cost of the spectroradiometer, the device needed to obtain the spectral signature. The objective of this study is to reach an intermediate goal, verifying that even with all the guarantees required, it is possible to develop an effective model with generalization ability in space and time (within the same campaign).

Árboles de decisiones / Decision trees

La última etapa en esta línea de investigación es la evaluación de la capacidad de los árboles de decisión (Gehrke 2006; Loh 2011; Ruß and Brenning 2010) para estimar la concentración de nitrógeno en planta, empleando para ello la reflectancia de la planta en unas pocas longitudes de onda. Esta investigación se realiza en las mismas condiciones que el estudio con las técnicas de reducción de dimensiones.

Los árboles de decisión evaluados no emplearán más de tres longitudes de onda (reflectancia), de esta forma no será necesaria la participación de un caro espectroradiómetro de campo para realizar la estimación del estado nutricional del cultivo, superando el problema que tiene el trabajo con las técnicas de reducción de dimensiones.

No todo cambio en la concentración de nitrógeno en la planta tiene un efecto sensible en la misma, existiendo por tanto cierta incertidumbre en el cálculo del plan de fertilización. En consecuencia estimar la concentración de nitrógeno en planta sin una precisión de varios decimales, tal y como consigue el laboratorio, no tiene efectos significativos en la gestión agrícola.

Hacer que la salida del árbol de decisión sea un nivel para la concentración de nitrógeno en lugar de un valor concreto puede suponer una mejora en su efectividad. Esto sería así si el algoritmo de clasificación, puntos de ruptura naturales (Jenks 1967), agrupa de tal forma que resulte más fácil encontrar rasgos espectrales distintivos para cada nivel, lo que facilitaría la tarea a los árboles de decisión.

The last step in this research is the evaluation of the capacity of decision trees (Gehrke 2006; Loh 2011; Ruß and Brenning 2010) to estimate the nitrogen concentration in plants, using for it the reflectance of the plant at a few wavelengths. This research is carried out in the same conditions as the study with the techniques for dimensionality reduction.

Decision trees include up to three wavelengths (reflectance), so it will not be necessary to have an expensive field spectroradiometer for estimating the nutritional status of the crop, overcoming the problem of the work with the techniques for dimensionality reduction.

Not every change in the nitrogen concentration has a significant effect on the plant, so there is some uncertainty in the calculation of the fertilization plan. Estimating the plant nitrogen concentration without a precision of several decimal places (as the lab gets) has not significant effects on farm management.

Making the output of the decision tree is a level for the nitrogen concentration instead of a specific value can mean an improvement in the effectiveness of the decision tree. This would be so if the classification algorithm, Jenks natural breaks (Jenks 1967), groups such a way that it is easier to find distinctive spectral features for each level, which would facilitate the task of the decision trees.

Interpretación espacial de los parámetros de la planta / Spatial interpretation of plant parameters

En la otra línea de estudio, el diagnóstico agronómico de los campos conocida la concentración de los nutrientes y otros parámetros (altura, verdor,...) de las plantas, se expondrán los trabajos con dos explotaciones agrícolas ubicada en centro Europa (Chequia), sembradas de trigo de invierno.

Lo primero es la identificación de un índice de barata, fácil y rápida determinación que permita una correcta estimación del desarrollo de las plantas. Ese índice puede suministrar valiosa información al servicio de la gestión agrícola y una referencia válida con la que comparar, mediante regresiones no lineales y validaciones cruzadas, las concentraciones de los nutrientes en la búsqueda de una relación con significación estadística fruto de un vínculo causa-efecto que pueda ser empleado en la toma de decisiones.

Dada la dificultad de trabajar con pequeños conjuntos de datos, se evaluará el uso de los factores espaciales (funciones de superficie y variables topográficas) para:

- Verificar la relación espacial entre las muestras obtenidas en el mismo campo.
- Realizar una validación espacial de las relaciones encontradas entre el índice de desarrollo del cultivo y los nutrientes.
- Identificar factores limitantes no-nutrientes (textura, orientación,...).
- Interpolar los datos obtenidos en el muestreo a todo el campo. Esto último es muy importante dado que es posible efectuar el diagnóstico apoyándose en un muestreo de bajo coste del campo y por ello la geoestadística no es una alternativa de garantía por las dificultades para obtener un variograma fiable (Oliver 2010).

The other line of study is the agronomic diagnosis of fields known the nutrient concentration and other plant parameters (height, green ...). Works in two farms located in Central Europe (Czech Republic) and sown with winter wheat will be discussed.

The first is the identification of an index with cheap, easy and quick determination, which allows a correct estimation of the development of the plants. This index can provide valuable information at the service of the agricultural management and a valid reference with which to compare, using nonlinear regressions and cross-validations, the concentrations of nutrients in the search for a relationship (statistically significant), result of a cause and effect relationship that can be used in decision-making.

Given the difficulty of working with small data sets, it will evaluate the use of spatial factors (surface functions and topographic variables) to:

- Check the spatial relationship between the samples obtained in the same field.
- Perform a spatial validation of the relationships found between the crop development index and the nutrients.
- Identify non-nutrient limiting factors (texture, orientation ...).
- Interpolate to the entire field the data obtained in the sampling. It is very important since it is possible to make the diagnosis relying on a low-cost sampling. Geostatistics is not an alternative with guarantees by the difficulties of obtaining a reliable variogram with a low-cost sampling (Oliver 2010).

Lo que se obtendrá con la lectura de esta tesis / What you get by reading this thesis

Con el índice de desarrollo del cultivo, los estudios de relación (índice de desarrollo del cultivo y nutrientes) y los análisis basados en los factores espaciales se compondría un sistema integral para el diagnóstico agronómico de campos que no precisaría de estudios previos, que podría ser implementado con los datos obtenidos en un muestreo de bajo coste del campo y que podría identificar factores limitante de toda naturaleza, no sólo déficit de nutrientes. Siendo lo mejor de todo que el diagnostico estaría siempre respaldado por evidencias estadísticas obtenidas en el mismo campo.

Con el estudio radiométrico del triticale se pretende determinar la efectividad real de los índices espectrales de vegetación y comprobar si en esas condiciones (amplio rango de condiciones de desarrollo y amplio intervalo fenológico) la minería de datos (técnicas de reducción de dimensiones, árboles de decisión y algoritmos de clasificación) puede mejorar los resultados de los anteriores. Como todo ello está referido al triticale de doble propósito, los valores obtenidos podrían determinar el umbral mínimo de eficiencia de la radiometría apoyada por la minería de datos al servicio de la agricultura de precisión.

The crop development index (CDI), the analysis based on spatial factors and the studies of the relationship between CDI-nutrients would compose a comprehensive system for agronomic diagnosing of fields that does not require previous studies. It could be implemented with data from a low-cost sampling of the field and it would identify limiting factors of all kinds, not only nutrient deficit. Being

the best of everything that the diagnosis would always be supported for statistical evidence obtained in the same field.

The radiometric study about triticale seeks to determine the real effectiveness of spectral vegetation indices and check whether in these conditions, a wide range of development conditions and phenology, the data mining (techniques for dimensionality reduction, decision trees and classification algorithms) can improve outcomes thereof. As all this is based on the study with the dual purpose triticale, the values obtained could determine the minimum level of efficiency of the radiometry and data mining at the service of the precision agriculture.

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Evaluating spectral vegetation indices for a practical estimation of nitrogen concentration in dual purpose (forage and grain) triticale

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Header

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Short title: Practical estimation of nitrogen concentration in triticale by spectral vegetation indices

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Abstract

There is an ample literature on spectral indices as estimators of the crop's chlorophyll concentration, and, by extension, of the nitrogen concentration. In this line, the suitability of 21 of these indices was evaluated as nitrogen concentration indicators for the dual purpose (fodder and grain) triticale (X *Triticosecale* Wittmack). The interval of interest was the one in that it would be possible to intervene to correct the deficiency of nitrogen (defined according to practical criteria); one peculiarity of this study is that it only develops a model for that period; more developments complicate the profitability, because the annual stability is not guaranteed and calibration studies are expensive. The results showed that, although there are significant correlations between the greenness indices and the crop's nitrogen concentration, for none of the spectral indices the relationship can reach acceptable values that encourage their use in the new techniques of precision agriculture of low cost. One solution for

improving the effectiveness and reduce costs could be to use the information contained in the spectral signature beyond what is easily explicable by biochemistry and biophysics, in other words, using data mining in the search for new spectral indices directly related to the concentration of nitrogen in plant and stable throughout crop development. At present, the squared correlation coefficient (R²) of the best fits reach 0.5 for the later phenological stages, this mark is reduced to 0.3 with an approach of low cost.

Additional key words: cereals; leaf reflectance; nutritional status; precision agriculture; radiometry; remote sensing

Resumen

Evaluación de índices de vegetación espectrales para la estimación de la concentración de nitrógeno en triticale de doble aptitud (forraje y grano)

Existe una extensa literatura que describe el potencial de los índices espectrales como indicadores de la concentración de clorofila en el cultivo y, por extensión, de la concentración de nitrógeno. En esta línea se encuentra este trabajo, donde se evalúa la idoneidad de los 21 índices espectrales más usados para realizar estimaciones en triticale (X Triticosecale Wittmack) de doble propósito (forraje-grano). El intervalo fenológico de interés se define siguiendo criterios prácticos, es aquel durante el cual se puede actuar para corregir una deficiencia de nitrógeno. Una peculiaridad es que sólo se desarrolla un modelo para todo ese periodo; más desarrollos complicarían la rentabilidad, ya que la estabilidad de los modelos no está garantizada y las calibraciones son costosas. Los resultados mostraron que, aunque existe correlación significativa entre los índices de verdor y la concentración de nitrógeno, para ninguno de los índices espectrales la relación alcanza valores que animen a su uso en las metodologías de bajo coste. Para mejorar la efectividad y reducir costes se podría usar la información contenida en la firma espectral más allá de lo que es fácilmente explicable por la bioquímica-biofísica, en otras palabras, usar la minería de datos en la búsqueda de índices espectrales directamente relacionados con la concentración de nitrógeno y estables a lo largo del desarrollo del cultivo. El coeficiente de correlación al cuadrado (R²) del mejor de los ajustes existentes alcanza un valor de 0,5 para los últimos estadios fenológicos, marca que se reduce a 0,3 al emplear una metodología de bajo coste.

Palabras clave adicionales: agricultura de precisión; cereales; estado nutricional; radiometría; reflectancia de la hoja; teledetección

Abbreviations used: aR² (adjusted correlation coefficient); NDVI (normalized difference vegetation index); p-value (statistical significance); R² (correlation coefficient); RMSE (square root of the mean square error)

Introduction

Reflectance measurements can be used to obtain the values of the most widely used spectral indices (reviewed in Ustin *et al.*, 2004) as indicators of chlorophyll concentration. These indices, together with the canopy radiative transfer models, allow one to estimate the state of the vegetation from satellite and aerial images. Our ultimate goal is to make this approach a reality in agriculture and the action plan begins with identifying the most appropriate spectral index and estimating the magnitude of its relationship with nitrogen concentration. This study assesses the potential of the methodology in easily reproducible conditions on farms. The immediate objective is to determine if the spectral indices keep the effectiveness reported by other authors when implementation costs are reduced (only a model for relating reflectance and nutritional status by campaigning on a stage with high variability), which is necessary to facilitate the transfer.

Some of the spectral indices commonly used as indicators of chlorophyll concentrations include corrections for the effect of the soil on the measurements of the canopy reflectance (Huete, 1988; Rondeaux *et al.*, 1996; Zarco-Tejada *et al.*, 2004), unnecessary precautions in this study because it works with reflectance measurements of the leaf.

This work is in line with that described by Heege *et al.* (2008). They related the measurements of greenness, obtained by sensors mounted on farm equipment, with the dose of nitrogen fertilizer. They used fluorescence and reflectance measurements, in the case of reflectance; they tested the determination of the red-edge inflexion point both numerically and empirically.

The work of Li *et al.* (2010), although similar to this one, differs in that in this study is limited to one the number of models that relate the spectral index and the nitrogen concentration in the plant throughout the development, instead of looking for relationships for specific growth stages, that is what has been done so far because the plant changes during its development (Marschner, 1995; Azcón-Bieto and Talón, 2003) complicate another approach.

With the dual purpose triticale, one has the possibility of allowing livestock to graze more than once without ruining the harvest. After each grazing by livestock the plant has to regenerate the above-ground part and with it the ability to synthesize chlorophyll, but the below-ground part is unaffected so that the plant's nitrogen absorbing capacity remains intact. The result is an imbalance in the first weeks after each cutting which is manifest in a yellowing of the plant. This is not a symptom of nitrogen deficiency, since there has been neither a decrease in the concentration of this element nor an interruption in plant growth. This characteristic is a major additional obstacle to the transference of radiometric technology to the dual purpose triticale case.

Material and methods

As part of a study at the "La Orden-Valdesequera" Research Centre aimed at determining the optimal combination of seeding density, number of grazing and doses of nitrogenous fertilizers for growing triticale (X *Triticosecale* Wittmack), the reflectance of the leaves throughout the growth of the crop was measured.

The experimental design was a split-split-plot with four replicates. The first factor was the seeding density (400, 500 and 600 plants m⁻²), the second the number of times the crop was cut to simulate grazing (0, 1 and 2 grazing by livestock) and the third the dose of nitrogenous fertilizer (0, 75 and 125 kg ha⁻¹). Each factor had three levels, so that there were 108 experimental plots in total, each of 30 m². The leaf reflectance measurements were made at 80, 117, 132, and 164 days after seeding (campaign 2009). Together with these measurements, crop samples were taken and sent to the laboratory for the determination of the concentration of total nitrogen by the Kjeldahl method.

The weather is a key factor in plant growth and climate variability is sufficient to cause changes in the evolution of the crop year after year; for this reason, more important than the number of days from sowing is to indicate the phenological stage in which was the plant. Table 1 shows the correspondence between the number of days after seeding, the crop's phenological stage and the description of growth stage.

Table 1 Correspondence between the number of days after seeding and the crop's phenological stage (triticale).

	Phenological stage			
Days after seeding	Zadoks scale	Feekes Scale	Description	
90	25	7-8	Stem elongation	
80	35 7-8	7-0	(5th node detectable)	
117	40	9	Booting	
132	46	10	Booting (flag leaf sheath opening)	
164	65	10.5.2	Anthesis half-way	

The growth stages were determined using the Zadoks (Zadoks *et al.*, 1974) and Feekes scales (Feekes, 1941; Large, 1954). On this matter illustrative charts can be found in the book of Rawson and Gómez Macpherson (2000).

The influence of each factor on the nitrogen concentration measured for each of the 108 plots on each sampling day was analyzed (it is unknown whether all the factors at all levels have an effect on the concentration of nitrogen in plant). The analysis of variance for factorial designs (statistical analysis that corresponds to the split-split-plot design) determines a grouping of the elementary experimental plots according to the nitrogen content on each of the four sampling dates. All calculations were done using R 2.9 (R Development Core Team, 2004).

The crop's spectral signature is sensitive to phenological changes; this is a good reason to test the relation between the spectral index and the nitrogen concentration for each sampling date. This approach suffers from a serious handicap; a commercial application is difficult since in that case calibration studies would be needed for each growth stage, which compromises the economic viability of this technique. This is the reason because in this work, the restriction that only one model should cover the entire period of interest was established.

On each sampling date, 20 leaves at random were collected in each of the 108 elementary plots. Ten estimates of the reflectance (each averaging 50 readings) were made of these samples, using the ASD FieldSpec 3 spectroradiometer for this. This device has a spectral range of 350–2500 nm, a sampling interval of 1.4 nm for the range 350–1000 nm and 2 nm for the range 1000–2500 nm, and a spectral resolution of 3 nm at 700 nm and 10 nm from 1400 nm to 2100 nm. Readings were performed using a plant probe plus leaf clip. The light source of the plant probe is a halogen bulb with a colour temperature of 2901±10 K.

For each of the different groups of elementary plots defined according to their concentration of nitrogen on each sampling date, the mean reflectance was calculated by averaging the readings taken in their respective elementary plots. The average spectral signature for each of the groups identified during the growth of the crop was then used to determine the value of each of the selected spectral indices given in Table 2.

The relationship between the different spectral indices and the nitrogen concentrations was evaluated by calculating the correlation coefficient squared (R^2), the adjusted squared correlation coefficient (aR^2), the square root of the mean square error (RMSE) and the statistical significance (p-value) of the model (analysis of the variance explained as against the residual). Figure 1 is a flowchart that summarizes the whole process.

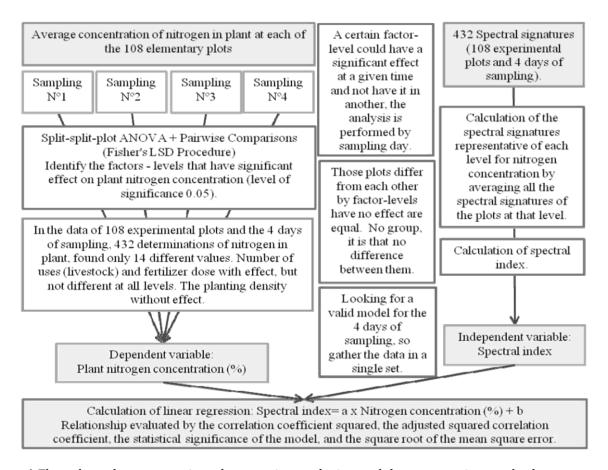


Figure 1 Flow chart that summarizes the experiment design and data processing methods.

Table 2 Spectral indexes related to the content in chlorophyll used

Spectral index	Formulation ¹	Author
Green NDVI ²	(R780-R550)/(R780+R550)	Gitelson and Merzlyak
		(1996)
Green reflectance	R550	Biochemical deduction
Logarithm of reciprocal	log(1/R737)	Yoder and Pettigrew-
reflectance		Crosby (1995)
Modified chlorophyll absorption	[(R700 - R670) - 0.2 * (R700 -	Daughtry et al. (2000)
in reflectance index	R550)]*(R700/R670)	
Modified red-edge normalized	(R750-R705)/(R750+R705-	Sims and Gamon (2002)
difference vegetation index	2*R445)	
Modified red-edge ratio	(R750-R445)/(R705-R445)	Sims and Gamon (2002)
Near infrared reflection	R800	Biochemical deduction
Normalized difference	(R800-R670)/(R800+R670)	Deering (1978)
vegetation index		
Pigment specific normalized	(R800-R675)/(R800+R675)	Blackburn (1998)
difference a		
Pigment specific normalized	(R800-R650)/(R800+R650)	Blackburn (1998)
difference b		
Pigment specific simple ratio a	R800/R675	Sims and Gamon (2002)
Pigment specific simple ratio b	R800/R650	Sims and Gamon (2002)
Ratio analysis of reflectance	R675/R700	Blackburn (1999)
spectra a		
Ratio analysis of reflectance	R675/(R650*R700)	Blackburn (1999)
spectra b		
Ratio of near infrared to green	R800/R550	Biochemical deduction
Ratio of near infrared to red	R800/R670	Biochemical deduction
Reciprocal reflectance	1/R700	Gitelson et al. (1999)
Red edge inflect point	(700+40)*{[(R670+R780)/2]-	Guyot <i>et al.</i> (1988)
	R700}/(R740-R700)	
Red reflectance	R670	Biochemical deduction
Red-edge NDVI	(R750-R705)/(R750+R705)	Sims and Gamon (2002)
Zarco-Tejada & Miller	R750/R710	Zarco-Tejada et al. (2001)

¹ R+number: reflectance at number nm. ²NDVI: normalized difference vegetation index.

Results and discussion

Table 3 shows that all the models, except the one developed for the modified chlorophyll absorption in reflectance index, explained a significant portion of the variance of the plant's nitrogen concentration, but in none of the cases the magnitude of the relationship was enough for developing a profitable methodology. The highest R² was 0.31, and corresponded to the green reflectance index.

This study determines the reduction in the effectiveness if one tries to estimate the concentration of nitrogen in the plant by a low-cost approach. The reduction is 38% (the value of R^2 is reduced from 0.5 to 0.31), a significant reduction received with a positive evaluation because of the complexity involved in developing a single model for different phenological stages and the enormous handicap which entails the double duality of the crop. It is understood that this reduction in effectiveness is the highest possible and that's not enough to discard the approach of a precision agriculture of low cost, at least remains to evaluate the potential of data mining in the exploitation of the information contained in spectral signature.

Table 3 Goodness of the fit between spectral indices and the concentration of nitrogen.

Spectral index	R ²	Adjusted	<i>p</i> -values	RMSE ¹
		R^2	for model	
Green NDVI ²	0.235	0.233	0.000	0.691
Green reflectance	0.315	0.314	0.000	0.653
Logarithm of reciprocal reflectance	0.179	0.177	0.000	0.715
Modified chlorophyll absorption in reflectance	0.008	0.006	0.065	0.786
Modified red-edge normalized difference	0.058	0.056	0.000	0.766
Modified red-edge ratio	0.047	0.045	0.000	0.771
Near infrared reflection	0.122	0.120	0.000	0.740
Normalized difference vegetation index	0.139	0.137	0.000	0.732
Pigment specific normalized difference a	0.123	0.121	0.000	0.739
Pigment specific normalized difference b	0.231	0.229	0.000	0.692
Pigment specific simple ratio a	0.115	0.113	0.000	0.743
Pigment specific simple ratio b	0.208	0.206	0.000	0.703
Ratio analysis of reflectance spectra a	0.027	0.025	0.001	0.779
Ratio analysis of reflectance spectra b	0.252	0.250	0.000	0.683
Ratio of near infrared to green	0.213	0.211	0.000	0.700
Ratio of near infrared to red	0.131	0.128	0.000	0.736
Reciprocal reflectance	0.226	0.224	0.000	0.695
Red edge inflect point	0.032	0.030	0.000	0.777
Red reflectance	0.173	0.171	0.000	0.718
Red-edge NDVI	0.156	0.154	0.000	0.725
Zarco-Tejada & Miller	0.134	0.132	0.000	0.735

¹ RMSE: square root of the mean square error. ²NDVI: normalized difference vegetation index.

The spectral signature of a leaf is extremely sensitive to the conditions affecting the leaf itself and to the conditions under which the measurements are made. These conditions vary considerably throughout the period during which it would be possible to act to correct a possible nitrogen deficiency in the crop, for this reason the models were specific to a growth stage, something that complicates the profitability and thus the transfer of technology, this study explores this field and its conclusion suggests that the cost of using a single model is not as high as could be expected.

In light of the results, exactly of the results of F test and associated p-value for significance of the model, one can say that the independent variables, spectral indices, are important in explaining the observed variation in dependent variable, concentration of nitrogen in plant. These indices have a

biochemical and biophysical basis, the existence of that relationship was expected, different is the magnitude of it, so small that makes one think about the weakness of using non-specific index for the concentration of nitrogen in plant.

It is confirmed that, in cultivating dual purpose triticale, calculations based solely on a greenness measurement, such as the green reflectance index (the index which gave the best correlation in this study), would lead to obtaining erroneous estimates of the nitrogen concentration.

The single model developed for the entire period of interest – from stem elongation (when tillering has ended) through booting and heading to flowering – gave lower correlations between the vegetation spectral indices and the crop's nitrogen concentration than those reported in similar studies in which different phenological intervals were modeled separately (Heege *et al.*, 2008; Li *et al.*, 2010). In particular, the value of R² was reduced by about 40%, from 0.5 for the final growth stages (Li *et al.*, 2010) to the value of 0.3 for the entire period of crop growth.

The techniques of precision agriculture have to reach to the cultivation of the dual purpose triticale. Since nitrogen's role in a plant is not restricted to be a component of chlorophyll and the spectral signature of the leaf is function of its composition and configuration, it has to be possible to derive new spectral indices which estimate nitrogen concentrations based on other variables besides of the greenness of the plant.

The results do not provide reliable indications of spectral features of those indices which best correlate with the crop's nitrogen concentration. Some authors, among others, the already cited Heege *et al.* (2008) and Li *et al.* (2010), have attempted to find relationships between the various spectral indices to explain their rank in terms of suitability (greater R²). The lack of correspondence between the different rankings might be considered a further reason for not addressing this issue.

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PCA versus ICA for the reduction of dimensions of the spectral signatures in the search for an index for the concentration of nitrogen in plant

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Header

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*Corresponding author: fernando.rodriguez@juntaextremadura.net | Phone: +34 924014071. Short title: Estimation of the nitrogen nutritional status by spectral analysis with PCA and ICA

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Abstract

The vegetation spectral indices have been widely used as estimators of the nutritional status of the crops. This study has evaluated if it is possible to improve the effectiveness of these indices to estimate the nitrogen concentration using dimension reduction techniques to process the spectral signatures. It has also demanded that the model is valid in a wide range of growing conditions and phenological stages, thus increasing the predictive power guarantee and reducing the implementation effort. This work has been done using an agronomic trial with dual purpose triticale (X *Triticosecale* Wittmack) whose design included plots with different planting densities, number of grazing and fertilizer doses. The spectral signatures of the leaves were recorded with the ASD-FieldSpec 3 spectroradiometer and the nitrogen concentrations were determined by Kjeldahl method. The factors with effect on nitrogen concentration were identified by the analysis of variance and pairwise comparisons and, then, the mean

spectral signature was calculated for each of the groups formed. The dimensional reduction was performed with both PCA and ICA. The analysis of the relationships between components and nitrogen concentration showed that only the components obtained with PCA generated a significant model (p=0.00) with a $R^2=0.68$. The best spectral vegetation index in this test, the reflectance in green, obtained a $R^2=0.31$. Although further confirmation is needed, this study shows that the PCA may be a viable alternative to spectral vegetation indices.

Additional key words: cereals; dual purpose triticale; independent component analysis; leaf; precision agriculture; principal component analysis; radiometry

Resumen

PCA versus ICA para la reducción de dimensiones de las firmas espectrales en la búsqueda de un índice para la concentración de nitrógeno en planta

Los índices espectrales de vegetación han sido ampliamente usados como estimadores del estado nutricional de los cultivos. En este estudio se ha evaluado si es posible mejorar la eficacia de esos índices para estimar la concentración de nitrógeno empleando técnicas de reducción de dimensiones para procesar las firmas espectrales. Además se ha exigido que el modelo sea válido en un amplio rango de condiciones de desarrollo y estados fenológicos, aumentando así las garantías de poder predictivo y reduciendo el esfuerzo de implementación. Se realizó un ensayo agronómico con triticale de doble aptitud (X Triticosecale Wittmack), en cuyo diseño se incluyeron parcelas con diferentes densidades de siembra, aprovechamientos y fertilización. La firma espectral de las hojas se registró con el espectroradiómetro ASD-FieldSpec 3 y la concentración de nitrógeno se determinó mediante el método Kjeldahl. Los factores con efecto en la concentración de nitrógeno fueron identificados mediante el análisis de la varianza y tests de comparación de medias; posteriormente se calculó la firma espectral media para cada uno de los grupos. La reducción de dimensiones se realizó tanto con PCA como con ICA. El análisis de las relaciones entre componentes y concentración de nitrógeno mostró que sólo las componentes obtenidas con PCA generaron un modelo significativo (p=0,00) con un R²=0,68. El mejor índice espectral de vegetación en esta prueba, la reflectancia en verde, obtuvo un R²=0,31. Aunque es necesaria una mayor confirmación, en este trabajo se muestra que el PCA puede ser una alternativa válida a los índices espectrales de vegetación.

Palabras claves adicionales: agricultura de precisión; análisis de componentes independientes; análisis de componentes principales; cereales; hoja; radiometría; triticale de doble aptitud

Abbreviations used: Adj R² (adjusted correlation coefficient); ICA (independent component analysis); MSE (mean square error); NDVI (normalized difference vegetation index); PCA (principal

component analysis); RMSE (square root of the mean square error); SNR (signal to noise ratio); SWIR (shortwave Infrared); VNIR (visible and near-infrared)

Introduction

The demand of nitrogen by the crop throughout its development is well known (Alaru *et al.*, 2004) and both the excessive and the deficit have a negative impact on production, operating costs and environmental conservation.

The technology available today can get huge volumes of information at a reasonable cost; the challenge is the correct interpretation of that information (Moran *et al.*, 1997). Reflectance measurements can be used to obtain the values of the most widely used spectral indices (Guyot *et al.*, 1988; Yoder and Pettigrew-Crosby, 1995; Gitelson and Merzlyak, 1996; Blackburn, 1998; Gitelson *et al.*, 1999; Daughtry *et al.*, 2000; Ustin *et al.*, 2004) as indicators of chlorophyll concentration. The suitability of these indices to estimate the concentration of nitrogen in plants is limited; Li *et al.* (2010) showed that the predictive power of these indices can reach a R²=0.5 for certain growth stages. Heege *et al.* (2008) reached higher values, but they linked the spectral signature with a dose of fertilizer applied and not with the nutritional status of the plant.

The work of Li *et al.* (2010) revealed one of the challenges to overcome, the poor spatial and temporal generalization of the models developed. Another difficulty was evidenced in the work of Rodriguez-Moreno and Llera-Cid (2011); the tests are conducted under conditions difficult to reproduce in real farms. In a real farm, for example, there isn't a panel of experts dedicated to calibrate the methodology, so the tasks of identifying acceptable cuts in the procedure and finding out the true effectiveness of the methodology are left to farmers.

In this context, only in the large farms (large areas) can bet strong for these new technologies, because the small improvements per unit area represent a significant increase in production and benefits, which compensated for the salary of specialist staff and equipment costs required for implementation. This is a sad reality as precision agriculture, besides trying to maximize profits, also seeks sustainability and protecting the environment (Moran *et al.*, 1997).

Studies, some of them six years old (Waheed *et al.*, 2006), have shown the high potential of radiometry and artificial intelligence in the field of precision agriculture, this work is in that line. The purpose of this study is to present a methodology which improves, in easily reproducible conditions on farms; the effectiveness of the methodologies based on the classical vegetation spectral indices and also offers greater guarantees of space-time generalization.

With the dual purpose triticale (X *Triticosecale* Wittmack), the crop used in this study, there is the possibility of letting livestock grazing on more than one occasion without ruining the final harvest. The plant after each grazing has to regenerate the above-ground part and with it the ability to synthesize chlorophyll, but the below-ground part is unaffected so that the plant's nitrogen absorbing capacity remains intact. The result is an imbalance in the first weeks after each cut, which is manifested by a yellowing of the plant. This is not a symptom of nitrogen deficiency, since there has been neither a decrease in the concentration of this element nor an interruption in plant growth.

The loss of greenness is not always related to a nutritional deficiency, this peculiarity, entailed by the crop chosen for the study, requires that the radiometric model is based on spectral features different from those used in many of the vegetation spectral indices such as the index of the reflectance in green. These new spectral features have to be more closely related to the concentration of nitrogen because they respond correctly under conditions in which the classical indices err.

There is no competition between old and new spectral features, it is a necessity dictated by the crop, when developing models for other cereals without the dual purpose both features can be integrated and thus obtain better levels of effectiveness.

One way to increase the guarantees of predictive power is limiting the number of models, only one model will be developed for the entire period during which it would be possible to correct the shortcoming nitrogen in the crop. The changes in the plant during its development (Marschner, 1995; Azcón-Bieto and Talón, 2003) complicate the development of generic models, but if that development is possible, then the model would provide greater guarantees, the Occam's razor is applicable. In addition, a unique development would reduce the participation of specialists in the implementation, which would reduce costs and would facilitate transfer of technology.

The huge volume of data obtained in a hyperspectral sampling is very complex to analyze and its processing has a high computational cost. For contexts such as these were devised dimension reduction techniques, which filter the noise, identify redundancies and reveal the structure hidden. The most widely used dimensional reduction techniques are principal component analysis (PCA) (Rao, 1964) and independent component analysis (ICA) (Hyvärinen and Oja, 2000). This study will examine whether the components identified by these techniques contain the information necessary to estimate, by a linear regression model and under the conditions described above, the nitrogen concentration in the plants.

The anticipated results would be evidences to support three hypotheses, the existence of features in the spectral signatures closely related to nitrogen concentration, the ability to develop models valid for a wide phenological range and the appropriateness of the dimension reduction techniques to process of the spectral signatures preserving the information on the nutritional status.

Material and methods

As part of a study at the "La Orden-Valdesequera" Research Centre (Badajoz, Spain) in order to determine the optimal combination of factors for the cultivation of the triticale, the reflectance of the leaves, at different stages of crop development, were measured.

The experimental design used was a split-split-plot with four replicates. The first factor was seeding density (400, 500 and 600 plants m⁻²), the second the number of times the crop was cut to simulate grazing (0, 1 and 2 grazing), and the third the dose of nitrogenous fertilizer (0, 75 and 125 kg ha⁻¹). Each factor had three levels, so that there were 108 experimental plots in total, each of 30 m². The leaf reflectance measurements were made at 80, 117, 132, and 164 days after seeding. Together with these measurements, crop samples were taken, which were sent to the laboratory for the determination of the concentration of total nitrogen by the Kjeldahl method. The correspondence between the number of days after seeding and the crop's phenological stage, along with his description, is presented in the

Table 1. The growth stages were determined using the Zadoks (Zadoks *et al.*, 1974) and Feekes, 1941 (Large, 1954) scales.

Table 1 Correspondence between the number of days after seeding and the crop's phenological stage

Days after	Phenolog	ical stage	Description
seeding	Zadoks scale	Feekes Scale	
80	35	7-8	Stem elongation
			(5 th node detectable)
117	40	9	Booting
132	46	10	Booting (flag leaf sheath opening)
164	65	10.5.2	Anthesis half-way

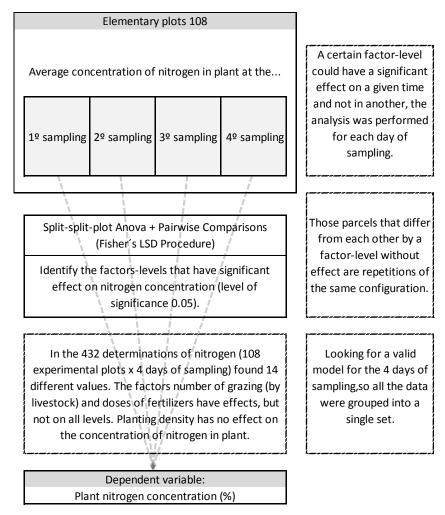


Figure 1 Flowchart of the statistical analysis for the concentration of nitrogen

In accordance with the experimental design, the influence of each factor on the nitrogen concentration measured for each of the 108 plots on each sampling day was analyzed (it is unknown whether all the factors at all levels have an effect on the concentration of nitrogen). The split-split-plot analysis of variance (ANOVA) and the pairwise comparisons, Fisher's LSD Procedure, determined a grouping of the plots according to the nitrogen concentration (p=0.05). Figure 2 is a flowchart explaining this analysis. This and the rest of calculations were done using R 2.9 (R Development Core Team, 2004).

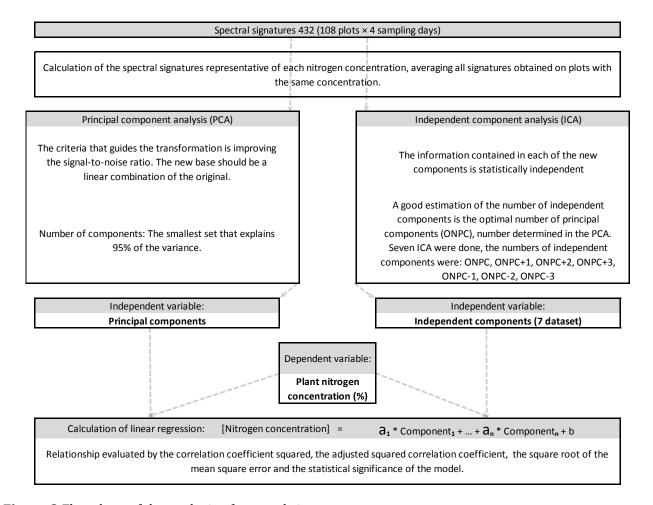


Figure 2 Flowchart of the analysis of spectral signatures

On each sampling date, 20 leaves at random were collected in each of the 108 elementary plots. Ten estimates of the reflectance (each averaging 50 readings) were made of these samples, using the ASD FieldSpec 3 spectroradiometer for this. This device has a spectral range of 350–2500 nm, a sampling interval (the spacing between sample points in the spectrum) of 1.4 nm for the range 350–1000 nm and 2 nm for the range 1000–2500 nm, and a spectral resolution (the full-width-half-maximum of the instrument response to a monochromatic source) of 3 nm at 700 nm and 10 nm from 1400 nm to 2100 nm. Readings were performed using a plant probe plus leaf clip. The light source of the plant probe is a halogen bulb with a colour temperature of 2901±10 K.

The reflectances for the wavelengths in which the transition between the spectroradiometer sensors (VNIR - SWIR1 and SWIR1 - SWIR2) occur were removed of the spectral signatures, regions where instrumental errors could be found.

For each of the different groups of elementary plots, formed according to their nitrogen concentration on each sampling date, the mean reflectance was calculated by averaging the readings taken in their respective plots. As the number of models has been limited to one, from this point all the pairs of nitrogen concentration - spectral signatures come together in one set, regardless of the date of sampling, since the model had to provide a correct estimate for all of them without knowing that information.

The dimension reduction techniques filter the noise, identify redundancies and reveal the structure hidden. There are different strategies; each employs different assumptions about the original components and the mixing process, mathematical assumptions that may not fit perfectly with the data set. This is the reason why two techniques, with statements so distant, have been tested.

The principal component analysis (PCA) searches for a new base, linear combination (this restriction simplifies the search) of the original base (in which the data were collected), that best expresses the data. For the PCA, the dynamics of interest is the one with better signal-to-noise ratio (SNR); this is the search criteria of the new base. Reducing the number of dimensions is got by eliminating noise and redundancy (Rao, 1964).

The independent component analysis (ICA) is the other technique that was tested. This dimension reduction technique seeks that the information contained in the new components is statistically independent (Hyvärinen and Oja, 2000). The ICA has been proved successful in many cases in which the PCA fails (Ozdogana, 2010).

The PCA returns as many components as inputs. In this study it was identified the smallest group of new components necessary to explain, at least, the 95% of the total variance, excluding other components; this is the way in which dimensional reduction was achieved. The ICA is different; one must indicate the number of independent components to generate. In this study the number of principal components (PCA) employed has been used as an estimation of the number of independent components (ICA) needed, performing several tests around that number.

It has built a linear regression model for each of the different sets of components generated (PCA and ICA) with nitrogen concentration (%). The goodness of fit of each model was evaluated by calculating the correlation coefficient squared (R²), the adjusted squared correlation coefficient (adjR²), the square root of the mean square error (RMSE) and the statistical significance (p-value) of the model (analysis of the variance). Figure 3 is a flowchart that summarizes the whole process.

The score to improve is 0.31, the value of R^2 obtained by the green reflectance index, which is the highest correlation found between the nitrogen concentration and the classical spectral indices. Calculation obtained with the same dataset that this study and performing the evaluation under the same conditions. The list of spectral indices analyzed in the comparative and other details of the study is in Rodriguez-Moreno and Llera-Cid (2011).

Results and discussion

The split-split-plot ANOVA (Table 2) and the pairwise comparisons (Fisher's LSD procedure) identified the factors with effect on nitrogen concentration (Level of significance in all tests of 0.05).

Table 2 Results of the split-split-plot ANOVA, factors with effect on nitrogen concentration

	Sampling					
Factor (cimple or	1st	2nd	3rd	4th		
Factor (simple or interaction)	Phenological stage					
interaction	Stem	Booting	Booting (flag leaf	Anthesis		
	elongation		sheath opening)	half-way		
Seeding density						
Number of cuts	_		*	*		
Dose of nitrogenous fertilizer	*		*	*		
Seeding density -	_					
Number of cuts						
Seeding density - Dose of	_					
nitrogenous fertilizer						
Number of cuts - Dose of	-	*				
nitrogenous fertilizer						
Seeding density -	_					
Number of cuts - Dose of						
nitrogenous fertilizer						

^{*:} effect on nitrogen concentration at the level of significance of 0.05.

It was observed that the factor seeding density had no effect at any time, the levels may not be appropriate or perhaps the effects were felt later.

The effect of the factor number of grazing was not analyzed in the first dataset, since the first cut was made after this sampling. In the dataset of the second and third sampling, with two levels (0 and 1 cut), it was determined that the factor number of grazing had effect on the concentration of nitrogen. The analysis of the fourth dataset, the first with three levels since the second cut was made after the third sampling, revealed that the three levels of the factor number of grazing had significant effect on plant nitrogen concentration.

The factor dose of fertilizer had effect on the concentration of nitrogen in all the datasets, but only in the fourth dataset the levels 75 and 125 kg ha⁻¹ had different effects. The fact that the effects of the two

higher doses of fertilizers do not differ is natural. The triticale takes the nitrogen from the soil along its development, but most absorption occurs in a developmental stage later than the dates on which the samplings were done (Lance *et al.*, 2007).

Those plots that differed only by a factor or level without effect were repetitions, so the representative value for the concentration of nitrogen and the spectral signature were obtained by averaging the data from plots with the same configuration. The 14 different nitrogen concentrations recorded in the 108 plots and the four days of sampling were: 1.02, 1.19, 1.22, 1.31, 1.36, 1.42, 1.52, 1.54, 1.64, 1.95, 2.32, 2.74, 3.14 and 3.40 percentage of nitrogen.

Cumulative variance explained by the first 10 components obtained using PCA reached 99.5% of the total variance. This percentage was considered sufficient, so only the first 10 components were taken into account in developing the linear regression.

Unable to make the same test to determine the appropriate number of components for the ICA, it was chosen to calculate 7 linear regressions (using 7 to 13 components). If the 99.5% of the variance of the reflectance could be explained with only 10 components in the case of PCA, ICA had to need something similar.

It has built a linear regression for each of the different sets of components generated (PCA and ICA) with nitrogen concentration (%). The goodness of fit of each model (Table 3) was evaluated by calculating the R^2 , the adj R^2 , the RMSE and the p-value of the model.

The best fit, R²=0.68, was reached in the linear regression with the components of the PCA. That result showed that the spectral signatures of crops meet the suppositions on the PCA is based (linearity in the change of base, higher variance means greater importance of the variable in the dynamics and that the principal components are orthonormal).

The winner model is presented in the Table 4. Except the fourth and ninth components, the rest were included in the model (Level of significance of 0.05). The eighth component is the one that gets the highest coefficient, but the seventh, the tenth and the second are close, so one cannot conclude that the concentration of nitrogen can be identified with a particular component, one must use the derived model.

This study provides evidences that data mining is an effective technique for analyzing the spectral signatures in the search for estimators of the nutritional status of the crop.

This work shows that the changes in the crop throughout its development are not sufficient to prevent the development of a single model. This means that the implementation of this methodology would require, at most, a calibration study per crop campaign. At this point it is worth recalling the high variability in the experimental plots in terms of growing conditions, which means that the effort to adjust the model could be valid for a large area.

Table 3 Goodness of all linear regressions made between the sets of components (PCA and ICA) and the nitrogen concentration (percentage of nitrogen)

Technique	Number of components	Significance of the model (p-value)	R ²	Adj R²	MSE	RMSE
ICA	7	0.19	0.02	0.01	0.62	0.79
	8	0.61	0.02	0.00	0.62	0.79
	9	0.12	0.03	0.01	0.62	0.78
	10	0.42	0.02	0.00	0.62	0.79
	11	0.48	0.03	0.00	0.62	0.79
	12	0.18	0.04	0.01	0.62	0.79
	13	0.33	0.03	0.00	0.62	0.79
PCA	10	0.00	0.68	0.67	0.20	0.45

Adj R^2 : adjusted correlation coefficient. ICA: independent component analysis. MSE: mean square error. PCA: principal component analysis. R^2 : correlation coefficient. RMSE: square root of the mean square error.

Table 4. Linear regression built with the components obtained with the PCA and the nitrogen concentration (percentage of nitrogen)

Coefficients	<i>p</i> -value
2.236	0.000
-0.013	0.000
-0.020	0.000
0.008	0.000
-0.001	0.551
0.009	0.001
-0.012	0.001
0.028	0.000
-0.053	0.000
0.003	0.742
0.027	0.028
	2.236 -0.013 -0.020 0.008 -0.001 0.009 -0.012 0.028 -0.053 0.003

In an evaluation, under the same conditions and with the same dataset, of the potential of spectral indices of vegetation to estimate the concentration of nitrogen in plant was determined that the best index was the reflectance in green, which reached an R^2 =0.31 (Rodriguez-Moreno and Llera-Cid, 2011). The results of this study placed the strategy with the PCA over the spectral indices such as NDVI. This is not surprising because it is not the first work that improves their effectiveness. An example is the result obtained by Waheed *et al.* (2006), which was able to develop a decision tree with a classification hit rate

above 90% in a similar experiment. The models developed by Waheed *et al.* (2006), with more than 5 years old, have been unable to replace the spectral indices of vegetation; the NDVI keeps its hegemony in the scientific and commercial uses.

The NDVI needs to be determined the reflectance at two wavelengths, the methodology presented in this article needs to be applied the complete hyperspectral signature. More information improves the estimates, but to overcome the NDVI, the simplicity and cost effectiveness are as important as the effectiveness.

The complexity of the new methodology could be reduced by identifying the wavelengths with greater weight in the components built into the model and developing with them a model that, instead of estimating the concentration of nitrogen, estimates if the plant is deficient in nitrogen. In that case one would only need to know the reflectance in a few wavelengths and the data processing would be easier.

Competing with the NDVI in terms of profitability would be possible with more studies supporting the greater effectiveness of this method in all scenarios and that is a valid methodology for large areas that only requires a calibration study per crop campaign. While both aspects do not improve, simplicity and profitability, the methodology presented will not end the hegemony of the spectral indices of vegetation.

Li *et al.* (2010) presented the model with more predictive power; in his development the spectral indices of vegetation and the brute force search were tested, by the difficulties of the brute force search one can say that the methodology presented in this article has a similar complexity. The models developed by Li *et al.* (2010) are specific for certain phenological stages and his best model reaches an R^2 =0.5, this work achieves a small improvement, R^2 =0.68, with a valid model for the whole period during which it could act to correct the deficiency in the crop.

It is very likely that this study has determined the lower threshold of efficacy, the dual purpose triticale supports the grazing by livestock throughout its development without ruining the final harvest; this makes it a special crop with additional difficulties for the development of radiometric models (details given in the introduction). It is hoped that the models developed for other cereals can get higher scores, but studies are needed to quantify it.

Developing this model has required the processing of over nine million data. In the case of developing a similar model with data taken in various scenarios (other locations, different weather, varieties, etc.) the data volume will grow exponentially, making it impossible to process, even for supercomputing centers. Proving that dimensional reduction techniques are effective is the first step required to initiate such studies.

The progress made has the limitation of requiring the spectral signatures of the leaves; an on-going investigation is going to determine if the model could be adjusted to operate with measures of vegetation canopy reflectance.

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A decision tree for nitrogen application based on a low cost radiometry

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Header

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Abstract

Fertilizer recommendations based on radiometry require studies to calibrate the relationships to scenario conditions; otherwise the effectiveness may be reduced. The objective of this study was to develop a decision tree to detect nitrogen deficiency with efficiency comparable to the analysis of the full spectral signature, with simplicity similar to a spectral index and valid over a wide range of development conditions and phenological stages. An agronomic trial with a dual purpose triticale (X Triticosecale Wittmack) was used in this study having different planting densities, number of grazing events (regeneration from defoliation) and nitrogen fertilization. At different phenological stages, the spectral signatures of leaves were recorded with an ASD-FieldSpec 3 spectroradiometer and the nitrogen concentrations were determined by the Kjeldahl method. Agronomic factors that affect the N concentration were identified using ANOVA; subsequently PCA was carried out on the set of spectral signatures representative of the groups formed according to nitrogen concentration. Linear regression was used to evaluate the relationship between the principal components and plant nitrogen concentration. Wavelengths with greater significance were used to construct a decision tree. The resulting decision tree defined for nitrogen using the Jenks Natural Breaks method had a success rate of 68.3%. The best spectral index had a $R^2 = 0.31$ while the estimate using the full spectral signature

reached a R^2 = 0.68. Although further testing is needed, this work shows the approach was able to successfully categorize nitrogen deficiency.

Keywords: Cereals - Classification algorithms - Leaf reflectance - Principal component analysis - Spectral vegetation indices

Abbreviations used: Adj R² (adjusted determination coefficient); ANOVA (analysis of variance); MSE (mean square error); NDVI (normalized difference vegetation index); PCA (principal component analysis); p-value (statistical significance); R² (coefficient of determination); RMSE (root mean square error); SNR (signal to noise ratio); SWIR (shortwave infrared); VNIR (visible and near-infrared)

Introduction

Models that relate spectral measurements with fertilizer rate need to be calibrated to scenario conditions to achieve the best fertilizer recommendations (Wood *et al.* 2003; Tian *et al.* 2009; Tian *et al.* 2011; Zhu *et al.* 2008; Y. Li *et al.* 2006). Interest in improving the efficiency and capacity of these relationships (generalization over space and time) is because they offer an immediate improvement in sustainability and profitability (Bongiovanni and Lowenberg-Deboer 2004).

Technologies for variable-rate nutrient applications based on prepared maps are commercially available. If such maps are appropriate, each land unit will receive the most appropriate treatment according to its characteristics (Llorens *et al.* 2010; Zhang *et al.* 2010), and frequently accompanied by a reduction of inputs and an increase in both production and quality. The nitrogen (N) demand of crops as they develop is well documented, as are the adverse effects that excessive and deficit nutrition have on production, operating costs and environmental conservation (Alaru *et al.* 2003; Gibson *et al.* 2007).

Technologies available today can generate huge volumes of information at a reasonable cost; the challenge is the correct interpretation of this information (Moran *et al.* 1997). Reflectance measurements can be used to obtain the values of the most widely used spectral indices (Vrindts *et al.* 2003; Dorigo *et al.* 2007; Broge and Leblanc 2001; Broge and Mortensen 2002; Li *et al.* 2008; Li *et al.* 2010) as indicators of chlorophyll concentration. The suitability of these spectral indices to estimate plant N concentration is limited as sometimes demonstrated under on-farm conditions (Li *et al.* 2010; Li *et al.* 2008). As such, there is need for calibration studies under scenario conditions (Wood *et al.* 2003; Yoder and Pettigrew-Crosby 1995; Zhu *et al.* 2008). The profitability of this approach is not high, but sensible (Auernhammer 2001; Robertson *et al.* 2007; Schellberg *et al.* 2008; Schroers *et al.* 2010). This increase in profitability combined with the simplicity of implementation has made spectral vegetation indices the approach of choice in scientific and commercial applications.

The alternative to spectral vegetation indices is the analysis of spectral signatures using data-mining techniques. The effectiveness can be superior, but the resulting models have a lower capacity to generalize space-time relationships and are more difficult and costly to implement (Li *et al.* 2010; Waheed *et al.* 2006; Goel *et al.* 2003; Rumpf *et al.* 2010; Ruß and Brenning 2010; Shao *et al.* 2009).

The available radiometric models are not ideal (Li *et al.* 2010; Waheed *et al.* 2006; Zhou *et al.* 2008; Yao *et al.* 2010). Improvements in both effectiveness and ability to generalize over space and time are desirable. Implementing these improvements is the goal of this research. The proposed methodology should be simple and require the lowest possible participation of specialists because any deployment cost will complicate the viability for precision agriculture.

Changes in plants during the growing season (Marschner 1995; Taiz and Zeiger 1991) complicate the development of general models, but if that development were possible, the resulting model would provide greater guarantees of predictive power. Moreover, it would reduce participation of specialists in the implementation phase, which would reduce costs and facilitate the transfer of technology.

The spectral signatures of the crop, coming from experimental plots with different planting densities, number of grazing events, N rates and growth stages are a set of data with more than nine million values. The analysis of such a data set is complex and computationally expensive, therefore PCA (Esbensen and Geladi 2009) was used. This dimension reduction technique reveals the hidden structure and eliminates redundant information and noise. This technique is suitable for this type of study because it simplifies the study of the relationship between the spectral signature and N concentration (Bajwa *et al.* 2004; Chen *et al.* 2009; Leon *et al.* 2003).

Linear regression was used to evaluate the relationship between the measured components and plant N concentration. Wavelengths with greater significance were used to construct a decision tree.

The expected response of the decision tree is the indication if additional N fertilizer is required by the crop; therefore, the target variable with which the decision tree had to be trained is the reclassified N concentration (adequate or inadequate level). There are four key crop development stages when it comes to sample collection. Each is associated with an optimal N concentration difference (Alaru *et al.* 2003) and thus the groups/levels used in the decision tree have been defined accordingly.

The Jenks Natural Breaks Classification method (Jenks 1967) has been used for reclassification. This algorithm groups all recorded N concentrations so that the variance within each group is minimal and the variance between groups is maximal. This algorithm was considered appropriate for this study because the treatments induce N concentrations that are distributed into natural groups (Jenks 1967) focused on the optimum for each phenological stage.

A decision tree is a nonparametric model in the form of a dichotomous key developed through a complex iterative algorithm. Its goal is to identify, from a training data set, the key features that allow predicting an attribute for a subject with a known probability of success. It is a technique that is included within the field of artificial intelligence and data mining. The recommendations of Breiman (1984) have been followed in the development of the decision tree.

Verato is the cultivar of dual purpose triticale (X *Triticosecale* Wittmack) used in this study. It supports the grazing of sheep, goats and pigs, which ends when livestock eat all the grass or when the crop reaches Zadoks 31 grow stage (Zadoks *et al.* 1974). In the case of early termination, it would be possible to have a second grazing (number of grazing events); even then this cultivar would provide a good harvest of grain. Plants regenerate the above-ground ability to synthesize chlorophyll after each grazing event, but the below-ground part is unaffected, so the N absorbing capacity remains intact. The result is a nutrient imbalance in the first weeks after each cut, which is manifested by a yellowing of the plant. This is not a symptom of N deficiency, since there has not been an interruption of plant growth; it is a quick restart that barely delays the physiological maturity date. The consequence is that the loss of

greenness is not always associated with a nutrient deficiency. As such, different spectral features are required than are typically used with more conventional vegetation indices, such as those that involve green reflectance. Any additional spectral features would hopefully capture aspects of the cereal cropping system that are not embedded within classical vegetation indices.

The objective of this research was to develop an innovative and effective spectral model for dual purpose triticale that characterizes the N status of the cropping system and thereby indicates the need for additional N fertilizer. Achievement of this goal would include developing data-mining protocols to identify and evaluate spectral features that are closely related to plant N concentration.

Material and methods

This work is a part of a study at the "La Orden-Valdesequera" Research Center (Badajoz, Spain) to determine the optimal combination of factors for the cultivation of a dual purpose triticale (X *Triticosecale* Wittmack, cultivar Verato).

Verato is a new winter triticale (X *Triticosecale* Wittmack) cultivar released in 2007 by the "La Orden-Valdesequera" Research Center. This cultivar of triticale continues to grow over the winter, has delayed bolting dates and reaches physiological maturity quite late. It shows better adaptation to cold areas, especially where soil fertility is lacking. This cultivar is very tall and in some cases it could have problems with lodging. It has high resistance against powdery mildew fungus (Blumeria graminis f.sp. Hordei), but unfortunately, it shows susceptibility to brown rust fungus (Puccinia recondita f.sp. Tritici), which influences the performance in areas where it is most common. It has an excellent tillering capability which affects yields that are usually low. It is a dual purpose cultivar (grain and fodder), mainly for its high ability for regrowth and tillering.

Spectral reflectance measurements were made using an ASD FieldSpec 3 spectroradiometer (Analytical Spectral. Devices, Boulder, CO, USA). This device has a spectral range of 350-2500 nm, a sampling interval (the spacing between sample points in the spectrum) of 1.4 nm over the range of 350-1000 nm and 2 nm from 1000-2500 nm, and a spectral resolution (the full-width-half-maximum of the instrument response to a monochromatic source) of 3 nm at 700 nm and 10 nm from 1400-2100 nm. Readings were performed using a plant probe with a leaf clip. The light source of the plant probe was a halogen bulb with a colour temperature of 2901 ± 10 K.

Crop samples were analyzed in the laboratory of the Research Center according to internationally accepted protocols. All calculations and statistical analyses were conducted using the software R 2.9 (R-Development_Core_Team 2008).

A split-split-plot design of experiment with four replicates was used. The first factor was plant density (400, 500 and 600 plants m^{-2}); the second factor was the number of cuts to simulate grazing (0, 1 and 2 cuts); and the third factor was N rate (0, 75 and 125 kg ha⁻¹). Each of the 108 experimental plots had an area of 30 m^2 .

Plant sampling in 2011 was done 80, 117, 132 and 164 days after sowing. On each sampling date, random leaves were collected in each of the 108 plots. The leaves in the top quartile of plant height were taken, leaves with the highest influence on measures of vegetation canopy reflectance; the reason

was to prepare the way for future research when working with vegetation canopy reflectance. Care was taken that the sample was representative of the entire surface of the experimental plot. Each sample was divided into two groups, twenty leaves were used in spectral analysis (ten measures, each an average of 50 readings, were made on these samples) and the rest was analyzed for the total N content using the Kjeldahl method.

The correspondence between the number of days after sowing and the crop's phenological stage, along with its description, is presented in Table 1. The growth stages were determined using the Zadoks (Zadoks *et al.* 1974) and Feekes (Large 1954) scales.

Table 1 Correspondence between the number of days after sowing and the crop's phenological stage

Days after	Phen	ological stage	Description
sowing	Zadoks	Feekes Scale	<u> </u>
	Scale		
80	35	7-8	Stem elongation (5th node detectable)
117	40	9	Booting
132	46	10	Booting (flag leaf sheath opening)
164	65	10.5.2	Anthesis half-way

The N treatments were designed so the plants would "always", "sometimes" and "never" be N deficient. Split-split-plot analysis of variance (ANOVA) and pairwise comparisons, Fisher's LSD Procedure, determined the classification of the plots according to the N concentration (level of significance in all tests of 0.05). The flowchart in Figure 1 illustrates this analysis.

Processing of the spectral signatures began by eliminating the reflectance of the wavelengths near the transitions between the spectroradiometer sensors (VNIR - SWIR1 and SWIR1 - SWIR2). The second step was to calculate the mean reflectance for each of the different N concentration groups. The number of models was limited to one, so from this point all the pairs of N concentration - spectral signature data came together in one set, regardless of the date of sampling, since the intended model needed to provide a reliable estimate of N concentration across a range of grazing situations, N rates, plant densities and growth stages.

Principal component analysis (PCA) searches for a new base, linear combination (this restriction simplifies the search) of the original base (in which the data were collected), that best expresses the data. For PCA, the dynamic of interest is the one with best signal-to-noise ratio (SNR); this is the search criteria of the new base. Reducing the number of dimensions is accomplished by eliminating noise and redundancy (Esbensen and Geladi 2009). The suitability of the technique for this work is supported by numerous studies (Bajwa *et al.* 2004; Chen *et al.* 2009; Leon *et al.* 2003).

Principal component analysis generates as many components as there are inputs. The smallest group of principal components necessary to explain 95 % of the total variance was identified. A linear regression model was generated to estimate N concentration (percentage) from the principal components (PCA). The goodness of the model was evaluated by calculating the coefficient of

determination (R²), the adjusted coefficient of determination (adjR²), the root mean square error (RMSE) and the statistical significance (p-value) of the model (analysis of the variance).

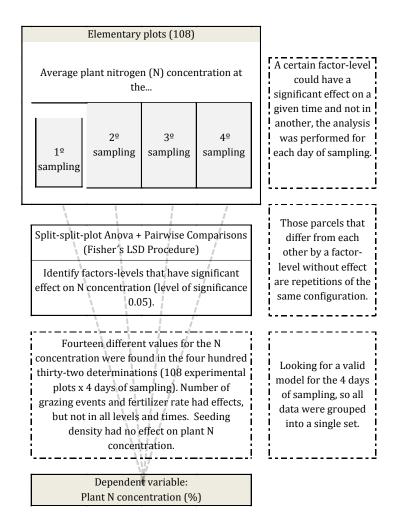


Figure 1 Flowchart of the statistical analysis of nitrogen concentration

This linear regression model was developed for a previous study (Rodriguez-Moreno and Llera-Cid 2011b). In that work this model was the final result, it is a significant model with a high coefficient of determination. In this work, it has been used as a method to identify the components that are significantly related to N concentration.

There are two PCA outputs, a set of principal components and a transformation matrix that projects the original data onto the new basis. The linear combinations that generated components significantly related to N concentration were extracted from the matrix to identify the two wavelengths having the greatest weight in each component. Treatments in this study ranged from N deficient to excessive, which encompasses optimal N concentration values for each sampling time during grazing and growth stage before maturity (Alaru *et al.* 2003).

The Jenks Natural Breaks Classification method (Jenks 1967) was used to classify N concentrations recorded during the four days of sampling. This algorithm minimizes the total sum of squared deviations by adjusting the thresholds for the different groups. Figure 2 illustrates the iterative process.

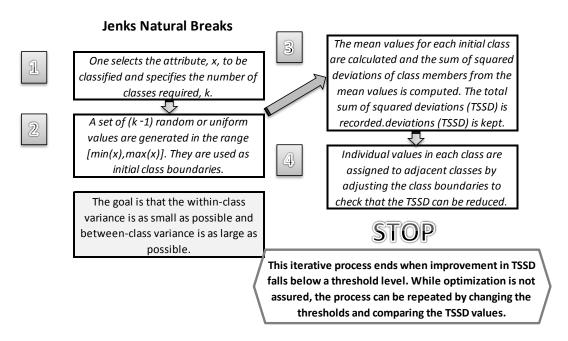


Figure 2 Flowchart of the algorithm to implement Jenks Natural Breaks

The recommendations of Breiman (1984) were followed in development of the decision tree. The decision tree classification algorithm was chosen because it was appropriate for the output variable. Gini's diversity index was applied as the split criterion. The weight of all observations was the same and the minimum number of observations that an impure node required before dividing was 10. All variables were considered in each division process. Once the decision tree reached its maximum size, the tree was pruned; the objective was to eliminate insignificant nodes of the training data set. This pruning minimizes the over-fitting problem and maximizes the predictive power of the model. Cross-validation was used in the evaluation of the decision tree; it allows obtaining a correct estimation of the predictive ability.

The decision tree needs to compete in simplicity with spectral vegetation indices that use reflectance values at two or three wavelengths for the calculation. For this reason, development of the decision tree was limited to a maximum of three wavelengths. The resulting decision tree has a combination of two or three elements (wavelengths) that are sensitive to plant N concentration. It should be recognized that the algorithm used to create the decision does not guarantee choosing the optimal set of input variables. Further, algorithms with a larger number of inputs variables may perform better. Figure 3 shows a flowchart that summarizes all the steps of the methodology.

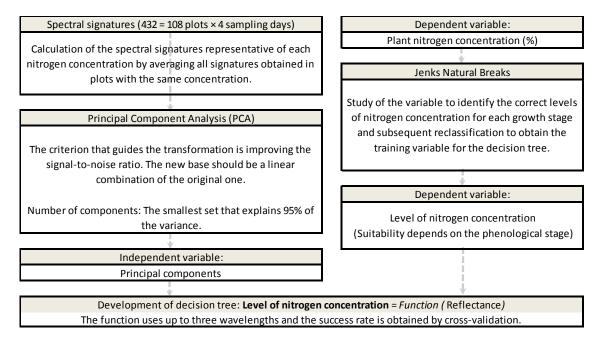


Figure 3 Summary of all steps of the methodology

Results

Split-split-plot ANOVA and pairwise comparisons (Fisher's LSD procedure) identified factors, simple or interaction, and levels with effect on N concentration (level of significance in all tests of 0.05). The factors are presented in Table 2. It was observed that planting density had no effect at any time, perhaps because the levels were not appropriate or the effects were expressed later.

The effect of grazing events was not analyzed in the first data set since the first cut was made after this sampling. In the second and third sampling data set, with two levels (0 and 1 cut), the factor had an effect on N concentration. The analysis of the fourth data set, the first one with three levels since the second cut was made after the third sampling, revealed that the three levels of grazing events had a significant effect on plant N concentration (Rodriguez-Moreno and Llera-Cid 2011a).

The N rate factor had an effect on all N concentration data sets, but only the 75 and 125 kg N ha⁻¹ levels had different effects within the fourth data set. Triticale takes N from the soil during its development, but most absorption occurs in a developmental stage later than the dates on which the samples were taken (Gibson *et al.* 2007); this is the reason why the effects of the two higher N rates did not differ.

Table 2 Split-split-plot ANOVA results, factors with effect on N concentration

Sampling	1º	2º	3⁰	4º
Phenological stage	Stem	Booting	Booting (flag leaf	Anthesis
	elongation		sheath opening)	half-way
Factor (simple or interaction)				
Planting density				
Number of cuts			*	*
Nitrogen rate	*		*	*
Planting density - Number of cuts				
Planting density - Nitrogen rate				
Number of cuts - Nitrogen rate		*		
Planting density - Number of cuts -				
Nitrogen rate				

^{*:} effect on nitrogen (N) concentration at level of significance of 0.05.

Plots that differed only by factors and/or levels without effect were repetitions, so the representative value for the N concentration and the spectral signature were obtained by averaging the data from plots with the same configuration. The 14 different N concentrations recorded during the four days of sampling in the 108 plots were: 1.02, 1.19, 1.22, 1.31, 1.36, 1.42, 1.52, 1.54, 1.64, 1.95, 2.32, 2.74, 3.14 and 3.40 % N. The result of the Jenks Natural Breaks Classification method application to this data set is provided in Figure 4.

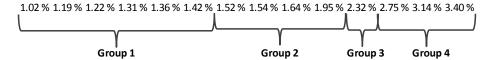
The variance explained by the first 10 principal components (PCA) reached 99.5 % of the total variance. This percentage was considered sufficient, so only the first 10 components were taken into account in subsequent analysis.

The procedure built a linear regression for the set of principal components and the N concentration (percentage). The goodness of the model, shown in Table 3, was evaluated by calculating the R², the adj R², the RMSE and the p-value of the model. The resulting model is presented in Table 4. Except for the fourth and ninth components, the rest were included in the model (level of significance of 0.05). The eighth component was the one that achieved the highest coefficient, but the seventh, the tenth and the second were close, so it is not possible to conclude that the N concentration can be identified with a particular component, it is necessary to use the derived model.

The result showed that the crop spectral signatures meet suppositions on which PCA is based (linearity in the change of base, higher variance means greater importance of the variable in the dynamic and that principal components are orthonormal).

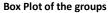
The two wavelengths with more weight in each of the 8 principal components significantly related to N concentration were identified in the transformation matrix (PCA). The reflectances at 350, 405, 420, 465, 495, 1300, 1480, 1670, 1690, 1705, 2010, 2055, 2170, 2180, 2210 and 2225 nm form the set of wavelengths sensitive to N concentration. All possible decision trees were generated using as input all combinations of two and three elements of this set of wavelengths. The best of them was the decision tree shown in Figure 5. Its evaluation, shown in Table 5, was calculated using cross-validation.

The 14 different nitrogen concentrations (%) recorded in the 108 plots and the four days of sampling



Classification by the Jenks Natural Breaks method

Statistic	GROUP-1	GROUP-2	GROUP-3	GROUP-4
Мах	1.42	1.95	2.32	3.40
3º Quartile	1.35	1.72	2.32	3.27
Median	1.27	1.59	2.32	3.14
1º Quartile	1.20	1.54	2.32	2.95
Min	1.02	1.52	2.32	2.75



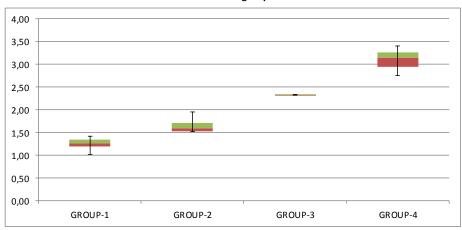


Figure 4 Natural groups obtained by classifying the nitrogen concentrations using the Jenks Natural Breaks Classification method

Table 3 Goodness of the linear regression built with the principal components (PCA) and the nitrogen concentration (percentage)

Technique	Number of	Significance of the model	R^2	Adj R²	MSE	RMSE
rechnique	components	(p-value)	N-	Auj N	MSE	KMSE
PCA	10	0.00	0.68	0.67	0.20	0.45

Adj R^2 : adjusted coefficient of determination. MSE: mean square error. PCA: principal component analysis. R^2 : coefficient of determination. RMSE: root mean square error.

Table 4 Linear regression built with the principal components and the N concentration (percentage)

	Coefficients	<i>p</i> -value
Constant	2.236	0.000
Component Nº1	-0.013	0.000
Component №2	-0.020	0.000
Component №3	0.008	0.000
Component №4	-0.001	0.551
Component Nº5	0.009	0.001
Component №6	-0.012	0.001
Component Nº7	0.028	0.000
Component Nº8	-0.053	0.000
Component Nº9	0.003	0.742
Component Nº10	0.027	0.028

The resulting decision tree needs only the reflectance at 350, 1670 and 2170 nm to reach a success rate (average of all groups) of 66.2 %. The number of cases in each of the four groups defined was not the same. If the success rate for the model was calculated using a weighted average by the percentage of cases in each group, then the model had a success rate of 68.3 %.

Table 5 Success rate of the decision tree

Group	1	2	3	4
Success rate	71.7 %	55.0 %	65.6 %	72.4 %
Success rate (simple average)			66.2 %	

Group	1	2	3	4
Weight of	27.8 %	13.9 %	22.2 %	36.1 %
each group				
Success rate			68.3 %	
Success rate (average weighted by the	e		68.3 %	

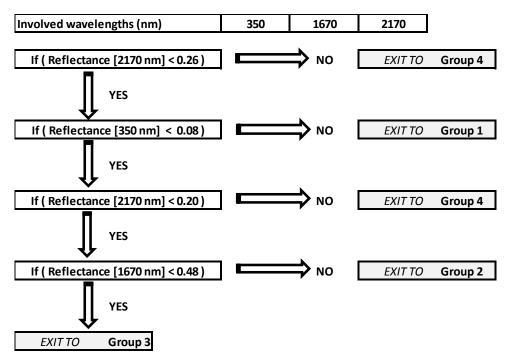


Figure 5 Decision tree for the nitrogen concentration created using reflectance at three wavelengths

None of the wavelengths traditionally used in the estimation of nitrogen (Rodriguez-Moreno and Llera-Cid 2011a) has been included in the decision tree. This can be explained by the cultivar used in the study, the dual purpose triticale, where the greenness of the plant is not always a good estimator of N concentration. The reflectance at 350 nm has been associated with the photosynthetic activity (Ray *et al.* 2007; Ren *et al.* 2006) and the reflectance at short-wavelength infrared (1670 and 2170 nm) is related to water stress (L. Zhang *et al.* 2012; Wang *et al.* 2010), which sometimes is related to the N concentration (Zhao *et al.* 2004). These references indicate what could be the main biological meaning of the wavelengths used.

The result of PCA showed that 95 % of the information contained in the spectral signature could be expressed with only 10 principal components. Reflectance values at different wavelengths are not independent of each other and therefore it is not always easy to describe a pure biological reason for the identified wavebands. Others have shown that the wavelengths used in the decision tree are directly related to the N concentration at different phenological stages (Li *et al.* 2010; Koppe *et al.* 2010).

The potential for spectral vegetation indices to estimate plant N concentration was evaluated. The test, based on the same data from the agronomic trial with triticale, determined that the best spectral index involved green reflectance, which reached a R^2 =0.31 (Rodriguez-Moreno and Llera-Cid 2011a). In this work, the proposed strategy performed better than spectral indices, such as NDVI. This has not been the first experience where the effectiveness of spectral vegetation indices has been surpassed. An example is the result obtained by Waheed *et al.* (2006), who were able to develop a decision tree with a classification success rate above 90 % in a similar experiment.

The linear regression built with the goal to identify the principal components sensitive to N concentration, Tables 3 and 4, had a R² of 0.68, which could resemble a success rate of 82.5 %. That value is slightly below the success rate achieved by Waheed *et al.* (2006). Major differences were expected for the peculiarities of a dual purpose triticale for having developed a model for a wider range of phenological stages and for the measures taken to increase the guarantees of predictive power.

Using only the reflectance at three wavelengths (success rate of 68.3 %, Table 5), instead of the full spectral signature (success rate of 82.5 %, Table 3), means a 14 % reduction in the success rate. The change also means employing a simpler model, probably with higher capacity to generalize space-time relationships. Such a methodology that is easier to implement, cheaper and that can be accomplished with a handheld device rather than a complex and expensive spectroradiometer could be sufficient.

Discussion

The high efficiency achieved in a complex scenario under rigorous evaluation has provided support for the hypotheses tested in this work. The proposed methodology is not comparable to that of NDVI or similar. Vegetation spectral indices have a solid biochemical-physical foundation and their usefulness can be tested quickly and cheaply. The foundation of the proposed methodology is statistical and therefore, the hypotheses involved need to be tested by many studies. The positive results in this test encourage continuing this line of research, which could improve the effectiveness and reduce the costs of implementation of radiometric techniques, thereby speed up the transfer to agriculture.

The resulting decision tree is simple; any electronic device could implement it, a simple device that operates along the reflectance reader of the wavelengths involved in the decision tree. In the case of the model developed in the trial for the triticale, the wavelengths are available only via expensive spectroradiometers, the device used in the experience, but the methodology is equally applicable to simple spectral signatures obtained with cheap spectroradiometers.

In section results, a biological justification of wavelengths involved in the resulting decision tree has been included. This is not a necessary step because the mathematical evaluation of the predictive power of the model is sufficient guarantee. Moreover, as this study has shown again, the information contained in the spectral signature of the crop is redundant so the identification of a clear biological meaning to each wavelength is unusual; wavelengths commonly respond to multiple factors, hence the need to use data mining in the processing of these signals.

The model is therefore as simple as a spectral index of vegetation, but with greater effectiveness when it comes to categorizing plant N status. The success rate is only 14 % lower than that of the method that uses the full spectral signature, but since it is achieved with a simpler model, equally effective for a wide range of development conditions and growth, it is likely that its capacity to generalize space-time relationships is greater, thereby overcoming the handicap noted above.

The results support the hypothesis of the existence of features in the spectral signatures that are closely related to N concentration. The results also demonstrate the appropriateness of dimension reduction techniques, decision trees and classification algorithms to process spectral signatures, preserving information on the nutritional status of the crop. Such confirmation could have considerable importance. Developing of this model required processing of over nine million pieces of data. In the case of developing a similar model with data taken from various scenarios (other locations, different weather, etc.), the data volume would grow so much that it would be impossible to process, even for supercomputing centers. The first step required to initiate such studies was to prove that the techniques are suitable for processing and analyzing crops spectral signatures, a data set that is large and complex.

A question that remains is the magnitude of the calibration necessary to use the resulting model in another scenario with the same success. The implementation of this methodology would require, at most, a calibration study per crop season. At this point, it is worth recalling the high variability in the experimental plots in terms of growing conditions, which means that the effort to adjust the model could be valid for a large area. Perhaps it is possible to design simple experiments to estimate the calibration parameters of the model, experiments that farmers could perform.

The resulting model is ready to operate in a wide range of conditions, but its effectiveness is unknown. Fortunately, it is a challenge that is faced with a large arsenal of modeling and analysis techniques (derivative of the reflectance with respect to the wavelength or the time, neural networks, genetic algorithms, multivariate adaptive regression splines, etc.). These techniques have already demonstrated their enormous potential to solve problems of similar nature. The result obtained in this work has been evaluated as satisfactory; this is the reason why these techniques, more powerful in some ways, but also more complex, have not been employed.

It is very likely that this study has determined the lowest threshold of efficacy for a dual purpose triticale that supports the grazing of livestock during its development, without ruining the final harvest; this makes it a special crop with additional difficulties for the development of radiometric models (details given in the introduction). It is expected that models developed for other cereals without a dual purpose can achieve greater effectiveness. This increase would be achieved by the combination of spectral vegetation indices and models developed using the proposed methodology. This needs to be proven and quantified, therefore further studies are needed.

The resulting model requires direct-contact radiometric measurements of plant leaves. The next step is to determine whether, with measures of vegetation canopy reflectance, it is possible to reproduce the results. If that were achieved, then it would be appropriate to experiment with a high-efficiency system in real-time for the identification of the plant N requirements.

Competing with vegetation spectral indices, NDVI or similar, in terms of profitability would be possible with more studies supporting the greater effectiveness of the models obtained using this methodology. This study has shown that there are models valid for large areas because they respond satisfactorily even for crops under different growth conditions and they only require a calibration study per crop season because the model can be valid for a wide range of phonological stages. While it is not satisfactorily resolved, the presented methodology will not end with the hegemony of vegetation spectral indices, although the resulting models have achieved higher efficacies in scientific works.

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Spatial interpretation of plant parameters in precision agriculture with winter wheat

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Abstract

This paper presents a methodology for the spatial interpretation of plant parameters, which is used to diagnose the status of winter wheat. The crop monitoring took place in the Czech Republic in 2010 in two fields using uniform crop management (52 and 38ha). The survey was carried out at BBCH30 phenological stage using a regular sampling grid with 150m distance between points (27 and 18points). The plant height and chlorophyll concentration (Yara N-Tester) were recorded and plant samples were taken to analyze the nutrients concentrations (N, P, K, Mg, Ca and S). A crop development index was developed from plant height and N-Tester values and compared with the results of plant analysis in order to determine the relationships, which were validated through spatial analysis. It may indicate the nutrients which limit plant grow at that stage. As a next step, the crop development index was compared with yield data to evaluate the success and stability in identifying the limiting factors. The method revealed that the limiting factors in the first field were potassium, calcium and nitrogen (in that order), nutrients significantly related to soil, climatology (surface functions) and relief. In the second field, the crop development index was not associated with any nutrient, but it was related to the topography (slope and moisture). Furthermore, it is found that in both cases the diagnoses were consistent with the DRIS diagnoses. The results show that if leaf analyses are complemented with the

characterization of crop development, it is possible to obtain successful diagnosis using statistical and spatial analysis.

Keywords: Cereals / Crop development (biomass and crop vigor) / Diagnosis and Recommendation Integrated System (DRIS) / Plant nutrition / Site specific crop management / Spatial analysis

Abbreviations used: DRIS (Diagnosis and Recommendation Integrated System); CDI (Crop development index); p-value (Statistical significance); R² (Determination coefficient); RMSE (Root mean square error); SF (Spatial factors);

Introduction

Diagnosis of the nutritional status of a crop identifies the treatment necessary to correct potential deficiencies and allows the crop to develop properly without input wastage (Barker and Pilbeam 2007; J. B. Jones 1998; Marschner 1995; Mengel and Kirkby 2001). Today, with the rise of precision agriculture it is necessary to repeat the diagnostic procedure in each land unit (Srinivasan 2006; Stafford 2007). This is why indirect methods which offer a rapid assessment of a crop's nutritional status are sought, and why they rely upon the spatial relationship between samples to interpolate the results (Oliver 2010).

As a result of agronomic trials, it has been possible to determine sufficiency ranges for the different nutrients of most crops (Marschner 1995; Rengel 1998; Reuter *et al.* 1998). Using other agronomic studies, faster but with a greater demand for computational requirements and statistical knowledge, it has been able to identify the relationships (ratios) between nutrients that characterize the plants of a particular crop which offer the best yield (Bailey *et al.* 1997a; Bailey *et al.* 1997b; Bailey *et al.* 2000; Beaufils 1973). Recent advances in this topic correspond to the identification of spectral features related to the nutritional status of the crop, resulting in the development of handsets that after a few minutes of reading in the field provide fertilizer recommendations (N-Tester of YARA International ASA, Germany).

Agronomic studies leading to the identification of rules for the interpretation of leaf analysis have a particular configuration (Alves Mourão Filho 2005; Jeong *et al.* 2009; Krug *et al.* 2010; Partelli *et al.* 2007; Soltanpour *et al.* 1995). It is not possible to experiment with all feasible configurations of crop development, which means that outside of that range of tested conditions, in real complex conditions, the adequacy of those rules of interpretation is unknown.

Although agricultural practices and crop development correspond with one of the cases for which a given set of interpretation rules were developed, the assessment of nutritional status will not be available at all times. The methodologies that work with sufficiency ranges identify the phenological stage of the crop on which to carry out the sampling and the plant part to be analyzed to proceed to diagnose (Marschner 1995; Rengel 1998). The methodologies that use nutrient ratios were presented as being more robust in this section, but experimentation has shown that the sensitivity, although lower, continues (Agbangba *et al.* 2011; Amundson and Koehler 1987; R. Beverly 1987; R. B. Beverly

1991; M. E. Sumner 1977). Indirect methods are calibrated by means of some of the methodology described above. So, these methods inherit the same problems (Arregui *et al.* 2006; Liu *et al.* 2003), to which it has to add the errors inherent in using an indirect measurement instead of a leaf analysis.

The interpretation of a set of leaf analysis from a given field should not be done individually because they are not independent samples. It is the reason why geostatistics can be used successfully in their extrapolation (Gholizadeh *et al.* 2009; Qian *et al.* 2009; Vieira and Gonzalez 2003). Studying the variability (differential development) of the crop at the field (Cao *et al.* 2012; Guo *et al.* 2010) might come to understand the causes. After deducting the diagnosis, the corrective treatment is obtained by combining agronomy, technology and economics.

A methodology that studies the spatial variability of the crop has to start by defining an index to quantify the crop development. In this study that index is defined as the product of the reading of N-Tester and the plant height in centimeters. Both are simple measurements related to a large number of determining factors in the development of cereals such as chlorophyll content (Jhanji and Sekhon 2011), the phenological stage (Escobar-Gutiérrez and Combe 2012), health status (Byamukama *et al.* 2012), water stress (S. Ma *et al.* 2012; Niu *et al.* 2007), salt stress (L. Zhang *et al.* 2012), competitive stress (Yenish and Young 2004) and productivity (Ivanova and Tsenov 2011).

The variance recorded by the crop development index (CDI) has to be caused by some factor. For example, the concentration of potassium is not right across the field. If that were to be the case, the study of the relationship between CDI and potassium concentration by regression and cross-validation (Draper and Smith 1981; Witten *et al.* 2011) would reveal a significant relationship whereby the potassium explains a certain percentage of the CDI variance. By reversing the process, one develops a diagnostic method for identifying the limiting factor for crop growth. However, it has to be accepted that the relationship with statistical significance implies a causal relationship that can be used successfully in agricultural management, a hypothesis shared by all the traditional methods.

Spatial variability in the concentration of nutrients, the CDI (in the above example, potassium deficiency explaining the CDI should, in turn, be explained by means of a gradient in the soil properties ...) and the crop yield are the result of the interaction between soils, climate, topography, anthropogenic activities and health incidents (Blandino et al. 2012; Fiez et al. 1994; Halvorson and Doll 1991; Kravchenko and Bullock 2000; L. P. Li et al. 2012; Miller et al. 1988; Patil et al. 2010; Sharma-Poudyal and Chen 2011; Wiik and Ewaldz 2009). The soil and climate may be unknown, but their effects can be successfully represented by the use of surface functions (Irmak et al. 2010; Jiang et al. 2010; L. Ma and Zuo 2012; Shi et al. 2012; C. C. Yang et al. 2004; Zandi et al. 2011). The effects of the relief have to be a function of topographic variables (elevation, slope, aspect, curvature and flow accumulation) (Fraisse et al. 2001; Pachepsky et al. 2001; Persson et al. 2005), which can be derived from a digital elevation model obtained through a simple differential GPS (DGPS). If agricultural management is uniform or known, only a health problem of the crop in its early stages, due to the spatial-temporal randomness of its occurrence (de Carvalho Alves et al. 2009; Demon et al. 2011; Jewell et al. 2009; B. Li et al. 2011; Meentemeyer et al. 2008; Plantegenest et al. 2007), would exceed the modeling capacity of the group formed by surface functions and topographic variables, known in this work as spatial factors (SF). Studies have taken place in which strategies close to these have been tested successfully (Akramkhanov et al. 2011; McBratney et al. 2003; Moore et al. 1993; Odeha et al. 1994; Park et al. 2001).

There are two reasons to study whether the concentrations of nutrients, the CDI and the crop yield are related to spatial factors. Firstly, it serves as a check on the diagnosis because if a nutrient is

identified as limiting but it is not related to spatial factors, it would have to be considered a problem with the data or a lack of spatial relationship between samples. Secondly, these relationships with the spatial factors allow the interpolation of the variables and, thereby, obtain variable application maps and crop yield maps for the entire field. Both results are very important because of the small numbers of samples needed for the implementation of this methodology. In a small data set, the results are sensitive to outliers and the interpolation is limited using geostatistics because the number and distribution of data does not allow identifying of a reliable variogram (Oliver 2010).

The aim of this study was to improve the interpretation of leaf analysis, complementing the traditional diagnostic with a spatial interpretation of plant parameters (SIOPP), which could provide own evidence for each scenario of the factor that is acting as limiting for the crop development. This can improve agricultural management, rationalize inputs, increase crop yield, reduce environmental impact and improve the profitability of farms, probably through the implementation of the new methodology in system decision support.

Materials and methods

Field experiments and data collection

The data used in this study were obtained from an experiment carried out in two fields in the South Moravian region of the Czech Republic: The field Pachty (48° 59′ N, 16° 38′ E) with an area of 52.5 ha is located on a plain (elevation 176 – 182 m) with an average annual temperature of 9.2 °C, precipitation of 483 mm per year and a predominant soil type described as chernozem. The field Haj (49° 15′ N, 17°06′ E) has an area of 37.8 ha and is located in hilly terrain (elevation 280 – 342 m) with a haplic luvisol soil type, average annual temperature of 9.25 °C and precipitation of 542 mm per year. In 2010, both locations were planted with winter wheat (fore-crop: sunflower at Pachty, spring barley at Haj) and the crop management was uniform within each field.

In BBCH 30 growth stage (Zadoks *et al.* 1974), plant samples were taken for analysis of nutrients in dry matter (content of N, P, K, Ca, Mg and S) according to the methodology valid in the Czech Republic (Zbíral 2005). Simultaneously with plant sampling, chlorophyll concentration using an N-Tester (YARA International ASA, Germany) and the height of plants were measured, they are plant parameters used in this study. The survey was done in a regular grid of $150 \times 150 \text{ m}$ (27 samples in Pachty, 18 in Haj) within a circle of 5 m of diameter at each sampling point (Figure 1).

To get information about the final production at both locations, yield sampling was carried out with the same point grid two weeks before harvest. Spikes were cut from an area of 0.2 m2 at two places within a circle of 5 m of diameter at each point of the 150 m sampling grid. The spikes were threshed in lab and yield was estimated as t. ha⁻¹.

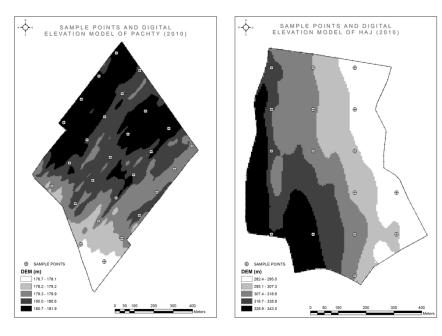


Figure 1 Sample points and digital elevation model in the field Pachty (left) and in Haj (right)

The digital elevation model was obtained using differential GPS (DGPS) measurement with Trimble Pathfinder ProXH in 2005 (Pachty) and 2009 (Haj). Elevation data were processed using ESRI ArcGIS to get the final DEM grid with resolution of 5 m per pixel and to calculate DEM derivatives (elevation, slope, curvature, aspect and flow accumulation).

Data analysis

The results of crop measurement (plant height and N-Tester) were used to establish the crop development index (CDI) using a simple equation: CDI = N-Tester * Plant height (cm). Both are simple measurements related to a large number of determining factors in the development of cereals (factors discussed above). Thus, this crop development index summarizes information on biomass and crop vigor and it can serve as an estimate of crop yield (Colla *et al.* 2008; Schepers and Holland 2012; Silvertooth and Norton 1999). Studying the index record would be possible to identify the threshold of viability, above which the intervention is cost effective in the field.

The variance of the CDI is an estimate of the spatial variability in the crop development (biomass and vigor). When working in a real agricultural field and with a low cost sampling, part of this variance is due to chance and sampling error, which could be estimated and used as threshold (it should also take into account the costs of adopting precision farming). If the coefficient of variation of CDI is below the threshold, the most likely explanation is that the crop development is uniform and therefore the best answer would be the realization of a pair of leaf analysis following a random sampling, averaging the results of laboratory, interpretation of analysis by traditional methods (sufficiency ranges or ratios between nutrients) and adoption of a uniform agricultural management in the whole field.

In case of rejecting the hypothesis of uniform crop development, it should be studied the relationship between CDI and spatial factors (SF). The SF (surface functions and topographic variables) represent the gradients in meteorology / climatology, soil and topography, which should be the natural cause of the spatial variability of CDI in the two fields (indications for other scenarios provided above).

If the CDI was not related to the SF, the hypothesis of spatial relationship between samples would have to be rejected and therefore it would be necessary to use the advanced techniques to delineate site-specific management units (Aimrun *et al.* 2011; Buttafuoco *et al.* 2010; Corwin and Lesch 2010; Guastaferro *et al.* 2010; Ortega and Santibáñez 2007; X. Zhang *et al.* 2010). This means using of the methods of precision agriculture such as the remote sensing, crop maps, electrical conductivity of soil, etc.

If the crop development was deficient and/or uniform or if there was not spatial relationship between samples, in any of the cases, the profitability of sampling and leaf analysis would be negative. This new methodology incorporates the above steps because they represent only a small additional effort and provide valuable information that helps to deduce the correct diagnosis. The improvements do not end here; reached the point where is evident the need for foliar analysis, the study of the CDI map helps determine the number and location of samples (the CDI map for the entire field is obtained using the model with the SF).

The fourth stage is the study of the correlation between the CDI and the concentration of each nutrient. This is studied independently by calculating the corresponding p-value and coefficient of determination (R²). Cross-validation was used for better assessment of the significance and magnitude of the relationships, the goal is to identify relations with predictive capacity (Antoniadou and Wallach 2000; Guisan and Zimmermann 2000; Muñoz and Felicísimo 2004; Steyerberg *et al.* 2001). The result of cross-validation is sensitive to the grouping because of the small number of samples (27 samples in Pachty, 18 in Haj), therefore 20 different random groupings were defined and the cross-validation was repeated for each of them (Cheng *et al.* 2010; Das *et al.* 2008; K. Yang *et al.* 2011). The result was the average of all evaluations. All calculations and statistical analyses were conducted using the software Matlab 2009b.

Exploring the regression model relating the CDI and a given nutrient can discover three important characteristics:

- It is possible to determine whether the nutrient is excessive (negative relationship with the CDI) or deficient (positive relationship).
- Comparing the coefficient of determination obtained by the different nutrients, it is possible to establish the order of importance, from the most important (which is responsible for the greatest variance in the CDI) to the least important.
- Knowing the cost of each fertilizer and studying the type of response between nutrient and CDI (linear, cubic, exponential ...), it is possible to determine whether that nutrient would get the largest increase in crop yield at lower cost.

If two or more nutrients are identified as limiting (significantly related to CDI), there is the possibility that their effects are related because the problem of one of them induces the problem in the other. In that case, the set of interrelated nutrients would present a high correlation and therefore it could be detected by evaluating the significance (p-value) and strength (R²) of the relationship between nutrients by cross-validation, the same process as described above. If two or more nutrients are linked by a relationship of cause and effect, one would have to identify which of those nutrients explains more

variance of the CDI and consult agronomic text to confirm that a problem with that nutrient may induce problems with the other nutrients involved.

In the fifth stage, the models that relate the concentrations of nutrients (those identified as limiting) with spatial factors have to be developed (as with the CDI). In both fields, there has been a uniform agricultural management and no health problem has been reported. In this scenario, if the crop development is not uniform (CDI is not close to constant), both the CDI as those nutrients responsible for its variability (limiting factors) have to be modeled as a function of spatial factors. If this requirement is not fulfilled, the diagnosis had to be rejected. The number of data involved is small and therefore sensitivity to outliers is very high.

Errors in sampling or analysis may alter the regression model between the nutrient and the SF, occasionally improving the goodness of fit and thus giving rise to a false identification as limiting. The same errors that very likely deteriorate the spatial structure of the data, which is why this fifth step serves as a check and has a capital importance. This procedure is inspired by the work of authors who have verified the spatial structure of the results obtained in different locations to evaluate the method used in the analysis (Basso et al. 2001; Grohs et al. 2009; G. Jones et al. 2010a, 2010b, 2010c). An illustrative figure of this diagnosis of outliers using spatial analysis is shown in Figure 2 and a flowchart summarizing the above is shown in Figure 3.

Diagnosis of outliers using spatial analysis

nagine twenty-four samples with two errors (below), one due to an unrepresentative sample and the other to a laboratory error, both lead to overestimate the concentration of the nutrient. There is a significant relationship with a high coefficient of determination (left). How could one know that this result is skewed by outliers? Statistical procedures, such as Cook's distance, would warn of two points with great weight in the but insufficient sampling Crop develop (biomass and vigor)

regression. Working with small dataset that will happen often and not always indicate outliers

plane (below), this is because 92% of the data is correct and practically constant. If attention is directed to the suspect data one would see that they have larger errors than the rest and that if the relationship was reevaluated by cross validation the coefficient of determination would fall

The lack of spatial coherence is the argument for rejecting the relationship between crop growth

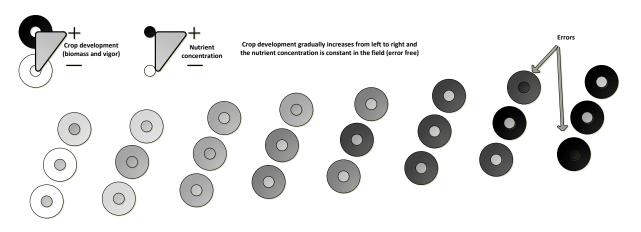


Figure 2 Explanation of how spatial analysis can help in identifying outliers

The models obtained in the final stage can be used in the interpolation of the data obtained in the sampling to the entire surface of the field, maps that could become variable rate maps. The latter is possible by identifying the concentrations of nutrients in the sample points where the highest levels for the CDI are recorded, the difference between these concentrations and the concentration at a given point, adjusted for the growth stage and plant density, determines the correction (dose of fertilizer). The interpolation using geostatistics is limited because the small number and distribution of samples, which not allows identifying of a reliable variogram (Oliver 2010), reason why these outputs in map form are very important.

Models relating the index of crop development (CDI), the concentrations of nutrients and the crop yield with the spatial factors (surface functions and variables topographic) have been developed using a stepwise linear and nonlinear regression (Draper and Smith 1981; Fox 1997; Hocking 2003; Rawlings *et al.* 1998). In case that the model is significant, it is evaluated by the cross-validation. In all stages of this research that used cross-validation, this has been done in the same way as described above and the same 20 sorting of the data were used.

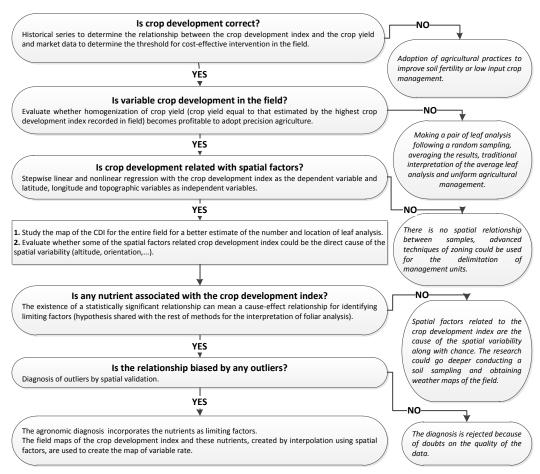


Figure 3 Flowchart summarizing the steps of the methodology spatial interpretation of plant parameters (SIOPP)

Evaluation

The evaluation begins with the interpretation of leaf analysis by the Diagnosis and Recommendation Integrated System (DRIS) (Beaufils 1973), using the norms for winter wheat obtained in the USA (Amundson and Koehler 1987), Canada (Amundson and Koehler 1987) and China(X. Li *et al.* 2005). The aim is to check whether the diagnoses obtained by traditional methods are consistent with those obtained by the spatial interpretation of plant parameters (SIOPP). There will also be a study made between the two fields to verify whether the relationship between the CDI and the nutrient balance index (NBI), obtained from the DRIS, is the expected one and if it is constant.

The second step in the evaluation is to check if the CDI is related to crop yield. An extraordinary event could change the existing spatial pattern during sampling, if that event has not occurred between sampling (BBCH 30 growth stage) and harvest, the CDI should be related to crop yield because none of deficiencies that could exist were corrected. For the same reason the nutrients identified as limiting have to be significantly related to crop yield, even the order of importance has to be kept. Quite the opposite happens if something occurs between sampling and harvest, then neither the CDI nor nutrient concentrations recorded in the sampling should be related to crop yield.

The last step is to study the relationship between crop yield and spatial factors. Regardless of whether anything has happened between sampling and harvest or not, the crop yield has to be able to be modeled by the spatial factors. That model would serve to create a crop yield map of the whole field and it could help to identify the incidence that could happen between sampling and harvest.

The foregoing is applied to the study presented in this article. In the case of implementing the recommendations obtained by this methodology, the evaluation procedure should be reversed. If the diagnosis is right and it has been put into practice then it is expected to get a uniform crop yield. If crop yield was close to constant over the entire surface, with the natural variations due to chance and sampling error, then there cannot be significant relationship with the CDI or the SF.

Comparison between the Diagnosis and recommendation integrated system (DRIS) and the Spatial interpretation of plant parameters (SIOPP)

Given the popularity of DRIS for interpreting leaf analysis, is understood that a presentation of the similarities and differences between DRIS and SIOPP will help better understand SIOPP. The information provided about DRIS in this section comes from an extensive literature review (Amundson and Koehler 1987; Arizaleta Castillo *et al.* 2006; Bailey *et al.* 1997a; Bailey *et al.* 1997b; Bailey *et al.* 2000; Beaufils 1973, 1975; Beaufils and Sumner 1977; R. B. Beverly 1991; Caron and Parent 1989; Gascho and Elwali 1984; Hartz *et al.* 2007; Letzsch 1984; X. Li *et al.* 2005; Mourão Filho 2004; Nachtigall and Dechen 2007; Parent 2011; Partelli *et al.* 2007; Raj and Rao 2006; Reis Jr 2002; Reis Junior and Monnerat 2003; Savoy Jr and Robinson 1990; Singh *et al.* 2012; Souza *et al.* 2011; M. Sumner 1977; M. E. Sumner 1977; Sumner and Beaufils 1975; Talkner *et al.* 2011).

Identifying the DRIS norms for a crop and geographical area usually begins by selecting a large number of fields. Several sampling in order to determine the concentration of nutrients during crop development and a final visit to record crop yield will be made in these fields. This huge data set (DRIS data set), representative of the most nutritious states and development conditions, is one of the strengths of the DRIS methodology for interpreting leaf analysis, the knowledge derived from it has great statistical support.

In the case of the spatial interpretation of plant parameters (SIOPP) is not necessary a study to identify the set of norms of interpretation, it only needs a small data set collected in the field that has to be diagnosed (the methodology is available to any crop as long as its CDI has been identified, which has been proved simple and is independent of the geographical area). The purpose is the agronomic diagnosis of that field; the recommendations will not be generalized to other field, so that the greater or lesser variance that is captured in this field is all that is needed. It will be analyzed to try to determine the factor or factors responsible for the spatial variability in the crop development (biomass and crop vigor).

DRIS dataset is processed through a combination of brute force (calculation of all possible ratios between the concentrations of nutrients, sometimes restricted to those pairs whose evolution during crop development follow the same trend) and statistics (each of these ratios between nutrients is evaluated using statistical tests to check for statistical significance that supports the use of this ratio to distinguish the crops with high and low yield).

That analysis method is not suitable for processing the data set obtained in a field because of the lower volume of data and variance. Since samples are not independent because they would come from the same field (it is unlikely that agronomic parameters vary randomly at small scale in a field), is possible to use regression models (linear and nonlinear), tests of statistical significance (ANOVA) and cross validation to identify the factor or factors responsible for the gradient in the crop development (biomass and crop vigor) registered in the field.

There is a common point of great importance between the two methodologies. The statistical methods used are different but the result is the same, identifying a statistically significant relationship between a factor (nutrient or other) and the crop development / yield. Both methods rely on that statistical relationship corresponds to a cause - effect relationship and therefore the crop yield can increase if one acts on the factor.

SIOPP uses an index of crop development (biomass and vigor) as reference instead of crop yield. This is the result of a necessity since SIOPP does not use information from a previous study and it has to provide a diagnosis at the time of sampling, when the crop yield is not available. The advantages of using an index of crop development are as follows:

The agronomic diagnoses will not be influenced by events that might occur between sampling and harvest.

Before spending resources on leaf sampling, it is possible to obtain a diagnosis which determines:

- If the expected crop yield makes cost effective the intervention in the field.
- If the crop is uniformly developed and therefore the best answer would be to adopt a uniform agricultural management.
- If there is spatial relationship between the samples, because otherwise advanced techniques of zoning for the delimitation of management units would be need.
- The CDI map for the field helps estimate the number and location of leaf samples, avoiding wasting resources.

Another difference between DRIS and SIOPP is the use of spatial factors (SF), it would be possible to study its incorporation into the DRIS but where the SF are essential and they give maximum benefit is in SIOPP. Thanks to them, five following objectives can be achieved:

- Study of spatial patterns.
- Diagnosis of outliers.
- Data interpolation.
- Help in identifying non-nutrient limiting factors.
- Support for the study of events that break the relationship between the crop development index and crop yield.

Results and discussion

Field Pachty

The coefficient of variation of the different nutrients ranges from 10 to 20% (Table 1), reason for determining the crop does not have a uniform development. This judgment is reinforced by knowing the coefficients of variation of N-Tester and crop height and it is confirmed by observing the variance in crop yield.

Table 1 Statistical summary of the plant parameters for the field Pachty

Pachty	N (%)	P (%)	K (%)	Mg (%)	Ca (%)	S (%)	N-Tester	Height (cm)	CDI	Yield (t.ha ⁻¹)
Mean	3.654	0.349	3.347	0.106	0.276	0.202	441.00	28.822	12795	7.963
St.dev.	0.382	0.055	0.350	0.020	0.052	0.021	52.637	3.900	2702	1.562
Kurtosis	1.287	-0.934	0.307	0.062	-0.685	0.687	-0.658	-0.300	-0.677	-0.611
Skewness	0.957	0.340	0.514	0.798	0.128	0.203	-0.268	0.420	0.048	0.544
Minimum	3.12	0.27	2.78	0.08	0.20	0.16	336.00	21.30	7796	5.60
Maximum	4.75	0.45	4.24	0.15	0.38	0.26	517.00	37.00	17786	11.06
CV (%)	10.45	15.70	10.46	19.10	18.84	10.36	11.94	13.53	21.12	19.62
n=	27	27	27	27	27	27	27	27	27	27

The convenience of using CDI in place of the reading of N-Tester or plant height was supported by the literature and it is confirmed by checking that the variance of the product is far superior to the individual variances, the CDI collects more information on crop.

The crop development is satisfactory because the readings of the N-Tester and the crop height are within the normal range for that growth stage determined by the historical data of the crop. The second requirement for the implementation of the methodology is that crop growth is not uniform, also satisfied given the coefficient of variation of CDI, about 21%. The third requirement is the existence of a significant relationship between the CDI and SF, which would confirm the spatial structure of the CDI and the causal role of SF. The coefficient of determination obtained proves the hypothesis, the requirement are meets.

The regression model between CDI and SF shows complicated interactions between surface functions and topographic variables, which results in a complex spatial pattern shown in Figure 4 (left). This map suggests increasing the number of samples in the field compared to that used in the

characterization of CDI and it provides indications of where they should be taken. In this experiment the number and location (regular grid) were kept. The result of this decision can be seen in the Table 2, the quality of the maps obtained for the nutrients and the crop yield are low, the suggestion was appropriate.

All requirements are met so it is possible to carry out a spatial interpretation of plant parameters (SIOPP), the results of the next step, the study of the relationship between CDI and nutrients, together with other studies, are shown in Table 2.

Table 2 Coefficients of determination among plant analysis results, CDI index, yield and spatial factors for the field Pachty obtained by cross-validation

Pachty	N (%)	P (%)	K (%)	Mg (%)	Ca (%)	S (%)	CDI	Yield (t.ha ⁻¹)
Yield	0.307**	0.033	0.552**	0.277**	0.428**	0.320**	0.515**	1
CDI	0.159^{*}	0.132	0.490**	0.123	0.311**	0.126	1	0.515**
Spatial factors	0.270^{*}	0.485**	0.170^{*}	0.274**	0.309**	0.376**	0.563**	0.168

The subscript numbers correspond to the coefficients of determination in the regression; they were not significant and therefore not proceeded to the cross-validation.

The concentrations of potassium, calcium and nitrogen are positively related to the crop development index; these are the nutrients that could be acting as limiting (Table 2). The correlations between them are shown in Table 3. All of them are significant but none reached a high value, the expected value for two nutrients linked by a relationship of the type inductor-induced. In winter wheat this relationship exists between nitrogen and sulfur (Järvan *et al.* 2012; Rasmussen 1996; Rasmussen and Douglas Jr 1992), having found between these nutrients a significant relationship with a coefficient of determination of 0.64.

Table 3 Coefficients of determination among nutrients significantly related to CDI obtained by cross-validation

leaf_N	leaf_K	0.24*
leaf_N	lea <u>f</u> _Ca	0.28**
leaf_K	leaf_Ca	0.22*

The K, Ca and N, in that order by percentage of variance explained of the CDI, are confirmed as limiting factors after checking that their concentrations are significantly related to spatial factors (Table 2). The results obtained indicate that the priority action to improve crop develop would be a variable-rate fertilizer application to correct the most likely limiting factor, potassium deficiency. It would also recommend correcting the deficiencies of calcium and nitrogen. Each nutrient has its own variable-rate application map derived from the interpolation to the entire surface of the CDI and the nutrient, using for this purpose the spatial factors. The concentration of the nutrient in the reference points, those in which the CDI reaches the highest values, is the level that the nutrient has to reach across the field, the

difference is calculated and corrected by phenological stage and crop density, the result is the fertilizer dose to be applied.

It is important to differentiate between the diagnosis and corrective treatment. With the same diagnosis the treatment varies depending on whether it wants to improve crop yield in the campaign or to find an efficient system. The results obtained by comparing the crop development index with nutrients (the identification of calcium as limiting) and the study of the maps of distribution of nutrients (Figure 4) warn about a problem with soil pH, so a correct treatment for potassium and nitrogen will force the plant development through the use of fertilizers (which will require the use of larger amounts of input each year). The alternative is to direct efforts to reach an efficient and sustainable soil (L-Baeckström *et al.* 2006; Miao *et al.* 2011; Míša and Křen 2001; Wienhold and Halvorson 1998).

Usually it chooses the first alternative, which explains why foliar analysis is a tool used in special cases where the crop yield in a given field has fallen to a point that investment in inputs is not profitable. In the diagnosis of this problem is where the methodologies for the interpretation of leaf analysis play a decisive role. Having an alternative to the sufficiency ranges and relationships between nutrients (DRIS and similar), which incorporates new techniques developed in recent decades (GPS, GIS ...), will increase the chances of success.

The nutritional balance index (NBI) with China norms reaches a 22.95, with USA and Canada norms the value stands at about 52 (Table 4). There is agreement between the DRIS diagnoses and the CDI to identify the existence of a severe nutritional imbalance in the development of the crop. Then the DRIS index for each nutrient will be studied to identify those responsible for the nutritional imbalance.

Table 4 Statistical summary of nutritional balance index (NBI), DRIS norms from USA, Canada and China for the Pachty field

Pachty	NBI (USA)	NBI (Canada)	NBI (China)
Mean	51.837	51.928	22.949
St.dev.	9.196	13.140	13.315
Kurtosis	-0.701	-0.058	-0.476
Skewness	0.461	0.728	0.672
Minimum	36.94	32.22	4.83
Maximum	71.67	84.05	52.82
CV (%)	17.74	25.30	58.02
n=	27	27	27

Each set of DRIS norms points to a different nutrient as limiting (Table 5). This lack of consensus highlights the need to obtain a set of DRIS norms specific for this scenario and prevent from identifying an incompatibility between DRIS and spatial interpretation of plant parameters (SIOPP).

Phosphorus is identified as limiting, with different severity, for the three sets of DRIS norms. That nutrient limitation was not identified as limiting by the methodology of spatial interpretation of plant parameters. Figure 4 (left) shows the crop reaches maximum levels of development in areas where the

concentration of P has minimum values. Given this evidence with statistical significance obtained in the data set of interest and the fact that crop yield is not significantly related to P (Table 2), the more plausible explanation is that the identification of P as a limiting factor is an error of the sets of DRIS norms used.

The rest of the DRIS diagnostic coincides with what is deduced by analyzing spatial. Potassium and nitrogen are limiting factors and the sulfur is not a problem in the two sets of DRIS norms, USA and Canada, where it is included in the calculations.

Table 5 Summary statistics of DRIS indices for nutrients with the norm from USA, Canada and China for Pachty

DRIS norms from		U:	SA			CAN	ADA			CHINA	
DRIS indices for	N	K	P	S	N	K	P	S	N	K	P
Mean	13,848	9,072	8,729	20,189	5,419	15,765	8,294	22,341	10,319	3,987	8,642
St.dev.	3,325	3,648	2,450	3,583	4,191	6,434	3,887	5,609	5,230	2,396	5,981
Kurtosis	-1,449	-0,426	-1,446	-0,252	-1,515	-0,494	-1,354	-0,317	0,325	-0,060	-1,171
Skewness	0,148	0,696	0,372	-0,011	0,054	0,625	0,219	-0,332	0,854	0,663	0,432
Minimum	8,726	3,344	5,402	13,290	-1,245	5,139	1,984	10,312	1,940	-0,004	1,155
Maximum	19,661	17,622	12,511	27,350	11,661	30,606	14,885	31,551	23,395	9,658	19,766
CV (%)	24,014	40,208	28,074	17,749	77,334	40,809	46,862	25,104	50,678	60,104	69,202
n=	27	27	27	27	27	27	27	27	27	27	27
				Perc	entage of	cases					
Position after		U:	SA			CAN	ADA			CHINA	
ascending sort	N	K	P	S	N	K	P	S	N	K	P
1º	0.00	7.41	81.48	11.11	100.00	0.00	0.00	0.00	0.00	29.63	70.37
2^{ϱ}	55.56	37.04	7.41	0.00	0.00	0.00	70.37	29.63	88.89	11.11	0.00
3^{ϱ}	44.44	55.56	0.00	0.00	0.00	92.59	7.41	0.00	11.11	59.26	29.63
4º	0.00	0.00	11.11	88.89	0.00	7.41	22.22	70.37		ı	1

Differential treatment was not applied so only if there had been some incidence from sampling to harvest, it could happen that crop development index was not related to crop yield. The coefficient of determination between development index and crop yield reached 0.51 (significant result evaluated by cross-validation), the hypothesis regarding the incidence was rejected and therefore the concentrations at BBCH 30 growth stage of the nutrients identified as limiting factors also have to be significantly related to crop yield and keep the order of importance (order by percentage of variance explained of the CDI). The coefficient of determination between the crop yield and potassium is 0.55, with calcium had 0.43 and with nitrogen 0.31 (Table 2).

In the field Pachty has been possible to deduce a successful agronomic diagnosis without the need of any prior study and without relying on the ability to generalize of a set of norms of interpretation obtained in another geographic area and / or with another crop.

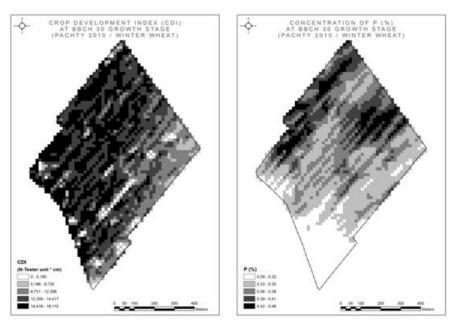


Figure 4 Interpolations based on spatial factors of the CDI (left) and of the concentration of P (right) in Pachty

Field Haj

The coefficient of variation for the different nutrients ranged between 3 and 8%, in that order of magnitude is unlikely that the crop was developing very heterogeneous (Table 6). This hypothesis is strengthened by knowing the coefficient of variation of the reading of N-Tester and the height of the crop, about half that recorded in Pachty, and it is confirmed by knowing the crop yield. The coefficient of variation of crop yield is situated 3 percentage points above the CDI; this is not an important variation but it reaches a magnitude more difficult to explain by random that the variability of CDI.

The convenience of using CDI in place of the reading of N-Tester or the height of the plant is again supported by checking that the variance of the product is higher than the variances of the factors, the CDI provides more information on the crop (Table 6).

Both the N-Tester readings and crop heights are within normal for that growth stage determined by the historical data. The crop development is satisfactory but the second requirement of the methodology, a heterogeneous development of the crop, only partially meets. The coefficient of variation of the CDI is about 10%, it is a low value in trials of this nature and it could be caused by noise or random. The doubt is solved by knowing that there is a significant relationship between the CDI and SF reaching a determination coefficient of 0.53. This means that there is spatial relationship between the samples and only 47% of the small variance cannot be explained by the SF, percentage of variance that can be caused by noise or random.

Table 6 Summary statistics of the plant parameters for field Haj

Нај	N (%)	P (%)	K (%)	Mg (%)	Ca (%)	S (%)	N-Tester	Height (cm)	CDI	Yield (t.ha ⁻¹)
Mean	5.000	0.492	3.641	0.112	0.488	0.328	584.78	29.428	17214	9.827
St.dev.	0.155	0.034	0.208	0.005	0.033	0.029	29.389	2.242	1632	1.232
Kurtosis	0.188	0.086	0.281	-0.436	-0.694	3.653	0.180	1.445	0.417	-0.094
Skewness	-0.688	-0.656	-0.454	-0.655	0.063	1.163	0.628	-0.001	0.176	0.764
Minimum	4.68	0.42	3.16	0.10	0.43	0.28	537.00	24.40	13786	7.97
Maximum	5.24	0.54	3.95	0.12	0.55	0.41	646.00	34.50	20528	12.32
CV (%)	3.09	6.94	5.71	4.73	6.84	8.86	5.03	7.62	9.48	12.54
n=	18	18	18	18	18	18	18	18	18	18

The relationship between the CDI and SF is supported mainly by a simple surface function, a decreasing gradient from southeast to northwest (Figure 5 left). In the next stage it will examine whether that gradient corresponds to some nutrient, but first is the sampling for leaf analysis. As in the field Pachty, the sampling for determination of CDI and foliar sampling is coincident, but unlike what happened in the field Pachty, in the field Haj the spatial pattern is simple (Figure 5 left) so the number and location of samples (regular grid) is correct and therefore the interpolations will have higher quality (the sampling could have been even smaller).

The requirements are fulfilled and therefore the results of the next stage of the methodology, the study of the relationship between CDI and nutrients, together with other studies, are presented in Table 7.

Table 7 Coefficients of determination among plant analysis results, CDI index, yield and spatial factors for field Pachty obtained by cross-validation

Haj	N (%)	P (%)	K (%)	Mg (%)	Ca (%)	S (%)	CDI	Yield (t.ha ⁻¹)
Yield	0.008	0.006	0.002	0.002	0.000	0.116	0.092	1
CDI	0.000	0.068	0.099	0.156	0.088	0.020	1	0.092
Spatial factors	0.455**	0.179	0.352*	0.246	0.288^{*}	0.538**	0.527**	0.758**

The subscript numbers correspond to the coefficients of determination in the regression; they were not significant and therefore not proceeded to the cross-validation.

None of the nutrient is significantly related to CDI and therefore there are no cross-correlations to study. There is not a large spatial variability of nutrients and therefore this result is not surprising, the question is whether the small spatial variability captured by the CDI is due to a gradient in soil properties, a gradient in moisture, etc. With the information available is not possible to identify the cause, the research could go deeper conducting a soil sampling and obtaining weather maps of the field. This information is not necessary for the purpose of this study, the facts are conclusive. None nutrient is identified as the cause of the low variability in the CDI and the crop is developing well and almost homogeneous. It is not possible to adjust the fertilizer plan in order to homogenize the crop yield. Under these circumstances the recommendation is to apply a generous and uniform fertilization.

The nutritional balance index (NBI) with China norms reaches a 24.59, with USA norms 20.41 and with Canada norms 15.20 (Table 8). The severity of nutritional imbalance is much lower than in Pacthy and that coincides with what is deduced from the CDI.

Table 8 Summary statistics of nutritional balance index (NBI), DRIS norms from USA, Canada and China, and CDI for Haj

Нај	NBI (USA)	NBI (Canada)	NBI (China)
Mean	20.411	15.197	24.592
St.dev.	6.182	5.315	5.501
Kurtosis	1.897	1.732	0.130
Skewness	0.309	-0.052	0.697
Minimum	6.24	3.09	16.71
Maximum	34.62	27.59	36.81
CV (%)	30.29	34.98	22.37
n=	18	18	18

The results provided by each set of DRIS norms mainly coincide with what they diagnosed for the field Pachty (Table 5 and 9). The fields Pachty and Haj differ in the soil, climate and topography, but they share the crop, winter wheat, and agricultural practices, good agricultural practices to get a high and uniform crop yield. Since agricultural practices follow the lead of agronomic studies conducted for years by the research centers of the Czech Republic, it is understood that partial matching between diagnoses is due to the mismatch of the DRIS norms for winter wheat is the same in both plots, skewing toward the same nutrient each set of norms, natural mismatch since none of them are calibrated to the conditions of the experiments.

The 53% of the small variability recorded in the crop growth is explained mainly by a function of surface (Figure 5 right and Table 7), the gradient does not coincide with the spatial distribution of P, N or K in the crop. The simplest explanation for that 53% of the variance is a gradient in the soil and / or climate (microclimate) on the field. The remaining 47% of the variance could be caused by random or an imbalance in the P, N, K, or combination thereof. In any case the magnitude of the problem is very small (47% of a small variance) to be sensed in a data set so small and to have a significant effect on crop yield, which is verified.

The common denominator between the different sets of DRIS norms and the diagnostic based on the spatial analysis is the lightness assigned to the problem responsible for the spatial variability of crop. The compatibility is in the key point because the crop yield shows that the crop grew well and almost homogeneous.

Table 9 Summary statistics of DRIS indices for nutrients with the norm from USA, Canada and China for Haj

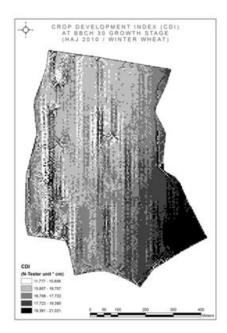
DRIS norms from		US	Α			CAN	ADA		CHINA		
DRIS indices for	N	K	P	S	N	K	P	S	N	K	P
Mean	6,530	-1,103	3,074	9,069	-1,750	-1,316	-1,555	8,573	13,560	5,824	5,208
St.dev.	1,612	1,795	0,980	3,883	1,326	2,880	1,852	5,036	2,584	1,339	1,866
Kurtosis	2,069	1,646	1,473	0,057	0,459	1,474	0,909	-0,280	-0,186	-0,250	2,805
Skewness	-0,431	0,763	0,003	0,115	-0,018	0,939	0,441	0,243	0,438	0,387	1,416
Minimum	2,348	-4,181	0,743	1,156	-4,699	-5,661	-5,387	-0,471	9,126	3,513	2,696
Maximum	9,480	3,484	5,110	16,548	0,457	6,105	2,488	18,623	18,634	8,568	10,507
CV (%)	24,686	162,677	31,866	42,822	75,750	218,860	119,073	58,737	19,054	22,989	35,837
n=	18	18	18	18	18	18	18	18	18	18	18
				Per	centage of	cases					
Position after		US	Α			CAN	ADA			CHINA	
ascending sort	N	K	P	S	N	K	P	S	N	K	P
1º	0.00	0.00	77.78	22.22	50.00	16.67	33.33	0.00	0.00	0.00	100.00
2º	100.00	0.00	0.00	0.00	38.89	5.56	55.56	0.00	16.67	83.33	0.00
$3_{\bar{o}}$	0.00	100.00	0.00	0.00	11.11	77.78	11.11	0.00	83.33	16.67	0.00
4º	0.00	0.00	22.22	77.78	0.00	0.00	0.00	100.00			

No significant relationship was found between CDI and crop yield (Table 7). The hypothesis of the occurrence of any incident between sampling and harvest is reinforced by observing that none of the concentrations of nutrients recorded in the sampling are related to crop yield.

The high yield of the crop did not suggest the occurrence of any incident between sampling and harvest. Now it is known that the spatial distributions of CDI and crop yield are not coincident, but it cannot be forgotten that their coefficients of variation are practically the same. With this information the most plausible explanation is that the ideal local configuration for crop development has changed, keeping the above scenario (what was good is not so good at harvest and that which was normal at sampling is good at end).

The last step in the evaluation is the study of the relationship between crop yield and spatial factors, a relationship that has to exist regardless of whether there has been (happened) any incidence between sampling and harvesting. Their relationship is significant and its coefficient of determination reaches 0.76, which was expected because it was known the simplicity of the spatial pattern of CDI and it is suspected that the incidence between sampling and harvesting alters the optimal relative position maintaining the same scenario.

Figure 5 shows the CDI (sampling) and the crop yield (harvest), both have been obtained using with the spatial factors. The comparison shows that the ideal local positions for crop development has changed from sampling to harvest; areas where the crop showed a better development during sampling do not correspond to areas of higher crop yield. This is not the expected effect of a health problem of crop (in addition it was not observed) and the soil parameters do not change in such a short period of time, the most likely factor is the climatology and within this the temperature and precipitation are classic candidates.



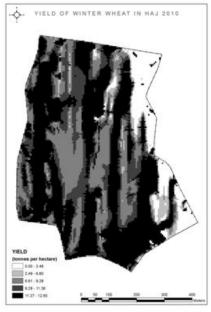


Figure 5 Interpolations based on spatial factors of the CDI (left) and the crop yield (right) in Haj

A period with an abnormal temperature could affect to the crop yield, even it could negate the relationship between CDI and crop yield, but it is not expected that it can change the ideal relative positions for the crop development. The other candidate is the precipitation. Up to sampling the crops was better developed in low areas, an intense precipitation in conjunction with a specific edaphology could change the ideal relative positions for crop development, making the upper and middle zones more suitable than the low, wherein the amount of water may be excessive.

From May to July the precipitation in 2010 was 228 liters per square meter higher than the average precipitation for that period, data obtained from the meteorological stations of the university and the meteorological service of the Czech Republic. This is an objective evidence to accept that in 2010 an incident happened between sampling and harvest, explaining the lack of relationship between the CDI and crop yield. Given this conclusion, a leveling of the land or improvement in the drainage would be advisable. It would homogenize crop yield and would decrease the effects of heavy precipitation. This finding proves that the verification phase of diagnosis can also provide valuable advice to farmers. This is another improvement that SIOPP incorporates, which helps to carry out integral agronomic diagnosis.

The spatial interpretation of plant parameters begins by identifying the variability in the crop development, then examines whether there is any robust statistical evidence that points to any of the factors as the cause of that variability in the field. The success of the diagnosis can be evaluated by the farmer with the data of the harvest, but this is not part of the methodology, it is a mechanism of evaluation. Sometimes it leads to the research of the incidence that annulled the relationship between CDI and crop yield. In this work it was necessary to carry out this research to show the success of the diagnoses obtained by SIOPP.

The argument that led to the identification of the precipitation (a campaign with abnormally high precipitation) as the cause of the incidence was not enough, that's why it was necessary to verify it by

studying weather and climate data. The identification of the incidence is an independent research and not always it will be easy to know what might be behind.

Conclusions

The identification of a simple crop development index (biomass and crop vigor) for winter wheat closely related to crop yield, even with uncertainties about its best formulation, improves agricultural management of fields because it enables the inclusion in the decision making process of an estimation of the crop yield (cost-effective intervention) and a measure of the spatial variability in the crop development (suitability of the use of precision agriculture and need for leaf sampling and analysis). Also provides a reference for the interpretation of leaf analysis which is not affected by events occurring between sampling and harvest the crop. Despite what might have been feared at first instant, the CDI is not biased towards a given nutrient or factor.

Using a stepwise linear and nonlinear regression, cross-validations and spatial checks has been possible to identify statistically significant relationships between crop development and factors (nutrient or other) with causal involvement. They can be used in agricultural management to improve crop yield. It has been possible to adapt the statistical procedures that support the other methodologies for interpreting leaf analysis to the data set obtained in a field, thus the diagnoses are supported by statistical evidence obtained in the same field (it does not require previous studies). This has been made possible by the inclusion in the analysis of spatial relationship between samples taken in the same field. The use of GPS, GIS and other tools of precision agriculture were not available at the time of development of the methodology for the interpretation of leaf analysis based on sufficiency ranges or relationships between nutrients. In this article is presented the natural evolution of those methodologies, although certain aspects have been modified to make them complementary.

The use of spatial factors (SF), surface functions and topographic variables, has allowed an effective evaluation of the spatial structure of the data and the identification of the factors (nutrient or other nature) affecting crop development. SF have also served for interpolation of the data obtained in sampling, which is very important when working with low-cost methodology, since the data do not allow identification of a reliable variogram and therefore geostatistics is not an alternative in this scenario. The cross-validation with repetitions and the aforementioned spatial verification are the other techniques that have been proven effective when working with small datasets (low-cost methodology).

Analyzing the relationship between the crop development index and the factor identified as limiting is possible to determine whether:

- The factor is acting as limiting by excess (negative relationship) or deficit (positive).
- The relative severity of the limitation (coefficient of determination).
- The response type (linear, exponential ...) that show the crop acting on the factor (function type).

This information together with the concentration of the nutrient in the points where the crop reaches its peak (maximum CDI) allows the development of an optimal fertilization plan.

The results presented in this article are important evidence for the spatial interpretation of plant parameters. Although further studies are needed to improve the formulation of the CDI and other

issues, from these pages are encouraged to increase minimally the sampling with the characterization of crop development and implement this methodology. It would be a convenient complement to the use of DRIS for the interpretation of leaf analysis, especially when the norms employed have not been specifically developed for the scenario (geographic area-crop).

The fundamentals of this approach are agronomy, statistics and spatial analysis. Probably too complex for many large agricultural fields where the binomial agronomy - remote sensing are giving great results. But because of the weaknesses of that binomial, those fields will have problems with the crop yield over time, moment in which leaf analysis may be the solution. If there alternative methodologies for the interpretation of the analysis, it will increase the chances of achieving a correct diagnosis.

This low cost methodology could be the first step in the adoption of precision agriculture by farmers (where the binomial agronomy and remote sensing is not profitable). Although statistical analyzes are complex, they are all implemented in software for statistical and spatial analysis, so its implementation would be in the scope of the soil laboratory or agronomic consultant.

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Resultados y discusión / Results and discussion

Estimación del estado nutricional del cultivo mediante radiometría / Estimation of nutritional status of the crop by radiometry

Veintiún índices espectrales de vegetación fueron evaluados, los 5 índices que alcanzaron los mejores coeficientes de determinación con la concentración de nitrógeno se muestran en la Tabla R1a.

Tabla R1a Los cinco mejores índices espectrales de vegetación en el estudio

Índice espectral	Formulación ¹	Autor	R ²	RMSE
Green reflectance	R550	Deducción bioquímica	0.315***	0.653
Ratio analysis of reflectance spectra b	R675/(R650*R700)	(Blackburn 1999)	0.252***	0.683
Green NDVI	(R780- R550)/(R780+R550)	(Gitelson and Merzlyak 1996)	0.235***	0.691
Pigment specific normalized difference b	(R800- R650)/(R800+R650)	(Blackburn 1998)	0.231***	0.692
Reciprocal reflectance	1/R700	(Gitelson <i>et al.</i> 1999)	0.226***	0.695

¹Formulación: Reflectancia a N (número) nm. R²: Coeficiente de determinación indicando el nivel de significación, todos con alfa igual a 0.001 (***). RMSE: Raíz cuadrada del error cuadrático medio.

El índice reflectancia en el verde alcanza un coeficiente de determinación de 0.315 y la raíz cuadrada del error cuadrático medio se sitúa en 0.653, lo cual supone el 27% del rango registrado por la concentración de nitrógeno en las 108 parcelas elementales y las 4 jornadas de muestreo. Con esa efectividad la mejora en la gestión agrícola sería sensible pero pequeña y por tanto no será una solución rentable para pequeñas y medianas explotaciones agrícolas.

Otros autores han realizado evaluaciones semejantes, en ellas se ha estimado que el coeficiente de determinación real (capacidad predictiva) que pueden alcanzar los modelos basados en índices espectrales se sitúa alrededor de 0.5 (Li *et al.* 2010a). La diferencia con esos estudios no pueden ser las condiciones de desarrollo del cultivo puesto que en todos se ha trabajado con un amplio rango para las mismas.

La peculiaridad del cultivo empleado en el estudio, el triticale de doble propósito, podría haber sido la causa de la reducción en la efectividad. El pastoreo del ganado obliga a un rebrote del cultivo y durante un tiempo se produce un desajuste entre desarrollo de la planta y síntesis de clorofila, ello se traduce en un amarillamiento que no alerta de la escasez de nitrógeno. En este contexto en el que el verdor de la planta no es siempre un indicador fiable del nivel de clorofila y dado que muchos índices espectrales de vegetación se apoyan en él (Feng *et al.* 2008), era previsible una reducción en la efectividad. El hecho de que el índice reflectancia en el verde alcance el mejor resultado prueba que los efectos del amarillamiento desaparecen rápidamente y que el doble propósito del cultivo no es la causa probable de la disminución registrada en la efectividad.

La otra diferencia con los estudios anteriormente citados es el hecho de haber desarrollado un único modelo para un amplio rango fenológico. Los resultados obtenidos sugieren que esta es la causa de la disminución en la efectividad, lo cual está respaldado por los estudios que alertaban de la pequeña capacidad de generalización espacio temporal de los modelos (Li *et al.* 2010a).

En la Figura R1a se proporciona una descripción de las longitudes de onda empleadas en los 5 mejores índices espectrales de vegetación. No es posible identificar una región del espectro que esté asociada con el éxito de los índices, eso abre la puerta a una exploración en la búsqueda de rasgos espectrales que puedan aunar esfuerzos para desarrollar modelos efectivos y generalizables, los modelos que se necesitan para que esta tecnología sea rentable en todas las explotaciones agrícolas.

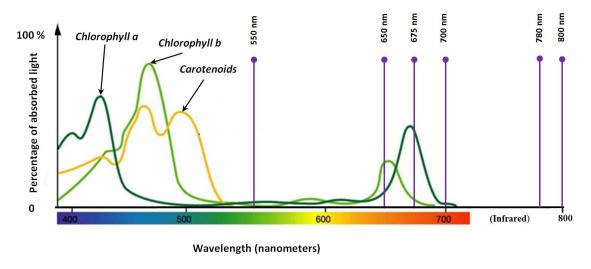


Figura R1a Diagrama ilustrando las longitudes de onda empleadas por los mejores índices espectrales de vegetación en el estudio

La firma hiperespectral del cultivo registrada durante el muestreo tiene un rango espectral de 350–2500 nm, un intervalo de muestreo (la separación entre dos puntos muestreados en el espectro) de 1.4 nm en el rango 350–1000 nm y 2 nm en el rango 1000–2500 nm, y una resolución espectral (el ancho total a la mitad de la altura de la respuesta del instrumento ante una fuente monocromática) de 3 nm a 700 nm y 10 nm en el rango 1400- 2100 nm.

Explorar este conjunto de datos mediante regresión múltiple no es posible por problemas de colinealidad. La Figura R2a muestra la reflectancia típica de la vegetación en función de la longitud de onda. La continuidad que se puede apreciar en la firma espectral evidencia que las reflectancias en las distintas longitudes de onda no son variables independientes. Sólo con que una de ellas fuese combinación lineal de las otras, el modelo de regresión sería irresoluble porque la matriz X'X sería singular (su determinante sería cero y no se podría invertir). En un experimento con datos reales la colinealidad perfecta es altamente improbable, pero es indiscutible que en los datos existe la llamada casi-colinealidad, dicho de otro modo, que algunas variables son "casi" combinación lineal de otra u otras. Esto se verificó comprobando que algunos coeficientes de correlación simple y múltiple entre las variables independientes están cercanos a 1, aunque no alcancen dicho valor.

Al existir casi-colinealidad en los datos la matriz X'X es casi-singular y su determinante no es cero pero es muy pequeño. Para invertir una matriz hay que dividir por su determinante y con un determinante pequeño la estimación de los coeficientes presentará problemas de precisión y será inestable. Además, como las varianzas (sus matrices) de los estimadores es proporcional a X'X, en presencia de colinealidad los errores estándar de los coeficientes serán grandes. La respuesta natural a este problema es el uso de las técnicas de reducción de dimensiones, las cuales fueron ideadas para trabajar en este contexto. A continuación se presentan los resultados obtenidos al aplicar el Análisis de componentes principales (PCA) (Shlens 2005) y el Análisis de componentes independientes (ICA) (Hyvärinen and Oja 2000).

Las diez primeras componentes principales obtenidas mediante el PCA concentran el 99.5% de la varianza total, lo cual es una confirmación del severo problema de colinealidad en los datos. Las reflectancias en las distintas longitudes de onda no son independientes entre sí y por tanto no es probable la existencia de una relación exclusiva entre la reflectancia en una región del espectro y un parámetro del cultivo. Una pequeña alteración de la planta podría llegar a afectar a una gran parte del espectro, esto puede explicar por qué se han identificado diferentes índices espectrales con los mismos parámetros del cultivo y por qué las evaluaciones de los mismos índices espectrales en otras condiciones no reproducen los resultados (Akiyama et al. 1996; Feng et al. 2008; Li et al. 2010a; Li et al. 2010b; Ustin et al. 2009; Zhu et al. 2006; Zhu et al. 2008; Zillmann et al. 2006).

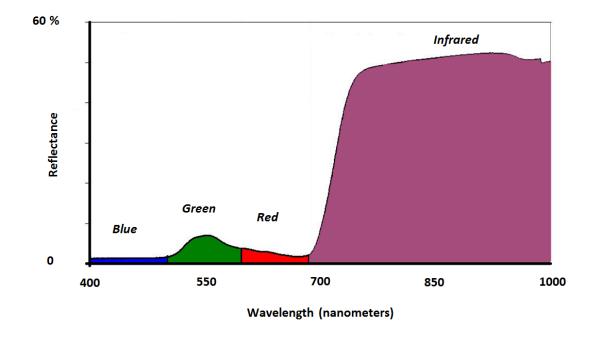


Figura R2a Firma espectral de la vegetación

Aún con ese primer resultado existe la posibilidad, aunque remota, de que el PCA haya perdido la información relativa al estado nutricional debido a un incumplimiento de alguna de sus suposiciones. Esto queda rechazado al comprobar que existe una relación significativa entre 8 de las componentes

principales y la concentración de nitrógeno en planta, alcanzando un coeficiente de determinación de 0.68.

Al haberse incluido en el modelo de regresión 8 componentes principales, ha de rechazarse el que hubiera sido el resultado deseado, la identificación de la deficiencia de nitrógeno con una determinada componente principal. En ese caso el estudio de la relación causa-efecto hubiera sido más sencillo y sólo se precisaría una parte de la firma espectral del cultivo para la estimación del estado nutricional. Dado el grado de conexión que existe entre las reflectancias en las diferentes longitudes de onda es natural que se haya necesitado una combinación de componentes para estimar un parámetro de la planta.

El buen resultado obtenido con el PCA hacía augurar un mal resultado con el ICA por los diferentes planteamientos que cada uno defiende. Los resultados confirmaron el pronóstico, el modelo entre las 10 componentes independientes y la concentración de nitrógeno en planta no resultó significativo (nivel de significación igual a 0.05) y el coeficiente de determinación se quedó en 0.02.

El resultado alcanzado mediante el procesamiento con el PCA de la firma espectral del cultivo supone una mejora respecto a los estudios realizados por otros autores (Heege *et al.* 2008; Li *et al.* 2010a; Li *et al.* 2010b), pero dado el alto coste del espectroradiómetro necesario para su implementación, el empleo de esta metodología está limitado a las grandes explotaciones agrícolas, donde la adquisición del equipo resultaría rentable.

Ahora que se conoce que es posible desarrollar modelos eficaces y generalizables en el espacio y en el tiempo, es momento de reducir su complejidad. Se probó con una combinación de árboles de decisión y fuerza bruta, lo cual condujo al desarrollo de un árbol de decisión que con sólo conocer la reflectancia del cultivo en 3 longitudes de onda (350, 1670 and 2170 nm), es capaz de estimar el nivel del nitrógeno en planta con una efectividad del 68%, resultado obtenido empleando validación cruzada.

Ninguna de las longitudes de onda tradicionalmente empleadas en la estimación de la concentración de nitrógeno en planta ha sido incluida en el árbol de decisión. La reflectancia a 350 nm ha sido vinculada con la actividad fotosintética (Ray et al. 2007; Ren et al. 2006) y la reflectancia en el infrarrojo de longitud de onda corta (1670 y 2170 nm) está relacionada con el estrés hídrico (X. Wang et al. 2010; Y. Y. Wang et al. 2010; Zhang et al. 2012), lo cual en ocasiones ha estado relacionado con la concentración de nitrógeno (X. Wang et al. 2010; Y. Y. Wang et al. 2010; Zhang et al. 2012). Lo anterior son indicaciones de los que podrían ser los significados biológicos de las longitudes de onda empleadas en el árbol de decisión, aunque solo es una explicación puesto que existen otros estudios que mostraron que esas regiones del espectro están directamente relacionadas con la concentración de nitrógeno en planta en diferentes estados fenológicos (Koppe et al. 2010; Li et al. 2010a).

Esta justificación biológica de las longitudes de onda implicadas en el árbol de decisión no es un paso estrictamente necesario porque la evaluación matemática del poder predictivo del árbol de decisión es garantía suficiente. La información contenida en la firma espectral del cultivo es redundante y por tanto la identificación de un significado biológico para cada longitud de onda es difícil. Lo normal es que la reflectancia en una determinada longitud de onda responda a múltiples factores, de ahí la necesidad de emplear la minería de datos para procesar estas señales.

Twenty one spectral vegetation indices were evaluated; the five indices that reached the top coefficients of determination with the nitrogen concentration are shown in Table 1Rb.

The green reflectance index achieves a coefficient of determination of 0.315 and a root mean square error of 0.653, which implies 27% of the recorded range for the nitrogen concentration in the 108 elemental plots and 4 sampling days. With that effectiveness the improvement in agricultural management would be sensible but small and therefore it will not be a profitable solution for small and medium farms.

Table 1Rb The five best vegetation spectral indices in the study.

Spectral index	Formulation ¹	Author	R ²	RMSE
Green reflectance	R550	Biochemical deduction	0.315***	0.653
Ratio analysis of reflectance spectra b	R675/(R650*R700)	(Blackburn 1999)	0.252***	0.683
Green NDVI	(R780- R550)/(R780+R550)	(Gitelson and Merzlyak 1996)	0.235***	0.691
Pigment specific normalized difference b	(R800- R650)/(R800+R650)	(Blackburn 1998)	0.231***	0.692
Reciprocal reflectance	1/R700	(Gitelson et al. 1999)	0.226***	0.695

¹Formulation: Reflectance at number nm. R²: Coefficient of determination indicating the significance level, all with alpha 0.001 (***). RMSE: Square root of the mean square error.

Other authors have made similar studies. They estimated that the real coefficient of determination (predictive power) of the models based on spectral indices is around 0.5 (Li *et al.* 2010a). The difference with these studies cannot be the conditions of crop development; all have operated with a wide range for the same.

The peculiarity of the crop used in the study, dual purpose triticale, could have been the cause of the reduction in effectiveness. Livestock grazing forces a crop regrowth and, for a time, there is a mismatch between plant development and synthesis of chlorophyll, it results in a yellowing which is not nitrogen shortage alert. In this context where the green of the plant is not always a reliable indicator of the level of chlorophyll and since many spectral vegetation indices rely on it (Feng *et al.* 2008), a reduction in effectiveness was foreseeable. The fact that the green reflectance index reaches the best result proves that the yellowing effects disappear quickly. The dual purpose of the crop is not the likely cause of the decrease in the effectiveness.

The other difference with previous studies is that a single model is developed for a wide range phenological. The results suggest that it is the cause of the decrease in effectiveness, which is supported by studies that warned of the small spatiotemporal generalization ability of the models (Li *et al.* 2010a).

Figure 1Rb shows a description of the wavelengths used in the top 5 spectral vegetation indices. It is not possible to identify a region of the spectrum that is associated with the success of the indices. That opens the door to exploration in the search for spectral features which can cooperate to develop effective and generalizable models, the models that are needed to ensure that this technology is profitable in all farms.

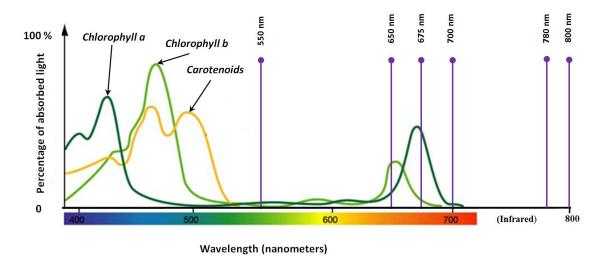


Figure 1Rb Diagram illustrating the wavelengths used for the best vegetation spectral indices in the study

The hyperspectral signature of the crop recorded during sampling has a spectral range of 350–2500 nm, a sampling interval (the spacing between sample points in the spectrum) of 1.4 nm over the range of 350–1000 nm and 2 nm from 1000–2500 nm, and a spectral resolution (the full-width-half-maximum of the instrument response to a monochromatic source) of 3 nm at 700 nm and 10 nm from 1400-2100 nm.

Exploring this dataset by multiple regression is not possible because collinearity problems. Figure 2Rb shows typical reflectance of vegetation as a function of wavelength. The continuity in the spectral signature proves that the reflectances at different wavelengths are not independent variables. If one of them was a linear combination of the other, the system of equations would be unsolvable because the matrix X'X would be singular (its determinant would be zero and it could not be reversed). In an experiment with real data the perfect collinearity is highly unlikely, but it is indubitable that in the data there is the called quasi-collinearity, in other words, some variables are "almost" linear combination of other. This was verified by checking the correlation coefficients (simple and multiple) between the independent variables, several are close to 1, but they do not reach that value.

There is quasi-collinearity in the data and therefore the matrix X'X is almost-singular and its determinant is not zero but is very small. A matrix is inverted dividing the matrix by its determinant and with a small determinant the estimation of the coefficients presents problems of accuracy and is unstable. Moreover, as the variances (their matrices) of the estimators are proportional to X'X, in the presence of collinearity the standard errors of the coefficients will be large. The natural response to this problem is the use of techniques for dimensionality reduction, which were designed to work in this context. The results of applying the Principal component analysis (PCA) (Shlens 2005) and the Independent component analysis (ICA) (Hyvärinen and Oja 2000) are presented below.

The first ten principal components obtained by PCA concentrate the 99.5% of the total variance, which is a confirmation of the severe problem of collinearity in the data. The reflectances in the different wavelengths are not independent of each other and therefore it is unlikely that there is a unique relationship between the reflectance in a region of the spectrum and a plant parameter. A small alteration might alter much of the spectrum of the plant; this may explain why different spectral indices

have been identified with the same crop parameters and why assessments of the same spectral indices in other conditions do not reproduce the same results (Akiyama *et al.* 1996; Feng *et al.* 2008; Li *et al.* 2010a; Li *et al.* 2010b; Ustin *et al.* 2009; Zhu *et al.* 2006; Zhu *et al.* 2008; Zillmann *et al.* 2006).

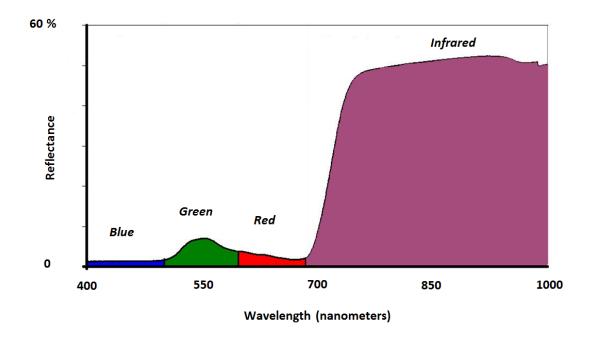


Figure 2Rb Vegetation spectral signature

Even with this first result there is a possibility, however remote, that the PCA has lost the information on the nutritional status due to the breach of any assumption. This was rejected after checking that there is a significant relationship between 8 principal components and the plant nitrogen concentration, relationship with a coefficient of determination of 0.68.

The regression model includes 8 principal components. The desired result, the existence of a relationship between a single principal component and the nitrogen deficiency, has to be rejected. If that had been the case, the study would have been simpler and it would require only a portion of the crop spectral signature for the estimation of the nutritional status. Given the degree of connection between the reflectances at the different wavelengths, it is natural requiring a combination of components to estimate a plant parameter.

The good results obtained with the PCA portended a poor outcome with the ICA; this is due to the different approaches that each defends. The results confirmed the prognosis, the model built with the 10 independent components and the plant nitrogen concentration was not significant (at the level of significance of 0.05) and the coefficient of determination remained at 0.02.

The result achieved by processing the spectral signatures of the crop by the PCA is an improvement on the studies of other authors (Heege *et al.* 2008; Li *et al.* 2010a; Li *et al.* 2010b), but given the high cost of the spectroradiometer necessary for its implementation, the use of this methodology is limited to large farms where the acquisition of the equipment would be profitable.

It is known that it is possible to develop effective and generalizable (space and time) models, now it is time to reduce their complexity. A combination of decision trees and brute strength was tested, which led to the development of a decision tree that just knowing the crop reflectance in three wavelengths (350, 1670 and 2170 nm) is able to estimate the level of nitrogen in plant with an effectiveness of 68%, a result obtained using cross-validation.

None of the wavelengths traditionally used in the estimation of nitrogen has been included in the decision tree. The reflectance at 350 nm has been associated with the photosynthetic activity (Ray *et al.* 2007; Ren *et al.* 2006) and the reflectance at short-wavelength infrared (1670 and 2170 nm) is related to water stress (X. Wang *et al.* 2010; Y. Y. Wang *et al.* 2010; Zhang *et al.* 2012), which sometimes is related to the nitrogen concentration (Zhao *et al.* 2004). These references indicate what could be the main biological meaning of the wavelengths used. Others authors have shown that the wavelengths used in the decision tree are directly related to the nitrogen concentration at different phenological stages (Koppe *et al.* 2010; Li *et al.* 2010a).

This biological justification of the wavelengths involved in the resulting decision tree is not a step strictly necessary, the mathematical evaluation of the predictive power of the model is sufficient guarantee. The information contained in the crop spectral signature is redundant and therefore the identification of a clear biological meaning for each wavelength is unusual; wavelengths commonly respond to multiple factors, hence the need to use data mining in the processing of these signals.

Diagnóstico agronómico mediante interpretación espacial de los parámetros de la planta / Diagnosis agronomic by spatial interpretation of plant parameters

Los resultados anteriores son una evidencia de que sería posible estimar eficazmente el nivel de los nutrientes en la planta de forma rápida y barata. Este avance por sí sólo no supondrá una gran ayuda para los agricultores puesto que falta una metodología para la interpretación eficaz de los niveles de los nutrientes en la planta.

Es posible realizar una detallada estimación (mediante radiometría, análisis foliares u otros métodos) del nivel de nutrientes en un campo agrícola y que eso no se traduzca en un aumento del rendimiento del cultivo. Esto podría suceder por diferentes motivos:

- 1. Porque sea un mal año en el que la mejor opción sea optar por una gestión agrícola de mínimos, cancelando el muestreo del cultivo porque no sería rentable. Es preciso poder estimar esta circunstancia en tiempo de muestreo.
- 2. Porque no exista estructura espacial en el cultivo, es decir, que los puntos de muestreo no sean buenos estimadores de su vecindad y por tanto los errores por la interpolación a toda la superficie arruinen la potencial mejora. Esto debiera ser investigado antes de emplear recursos en el muestreo del cultivo. Podría ser necesario el empleo de técnicas de delimitación de zonas de gestión.
- 3. Porque las normas para la interpretación de los niveles de nutrientes (rangos de suficiencia o relaciones entre nutrientes) no sean específicas del cultivo área geográfica y por tanto no sean eficaces. Diferentes trabajos mostraron la limitada capacidad de generalización.

4. Porque suceda algún evento entre el muestreo del cultivo y la cosecha, el cual afecte negativamente al rendimiento del cultivo. En ese caso ese evento debiera ser identificado para aumentar el conocimiento y ser capaces de evitarlo en el futuro.

Los resultados mostrados en el cuarto artículo que compone esta tesis responden a todas las cuestiones anteriores.

El índice de desarrollo del cultivo (CDI) mostró recabar más información sobre el estado del cultivo que la altura o el NTester de forma independiente, resultó ser un buen estimador de la variabilidad espacial del cultivo en ambos campos y en el campo Pacthy fue buen estimador del rendimiento del cultivo. El CDI no fue buen estimador de la producción en Haj porque entre el muestreo y la cosecha llovieron 228mm por encima de la media, incidencia que alteró el desarrollo del cultivo, conocido esto se evidenció que el CDI es un eficaz estimador del rendimiento del cultivo, pudiendo llegar a determinarse umbrales de viabilidad para el mismo. Si el cultivo no alcanza ese mínimo en el momento del muestreo la intervención en el campo no es rentable, lo que responde al primer punto de los mencionados anteriormente.

Para comprobar la estructura espacial se estudió la relación entre el CDI y los factores espaciales (funciones de superficie y variables topográficas), encargados de representar los factores que podrían causar la variabilidad espacial. En ambos campos se comprobó que existía una estructura espacial, dejando al azar y al error de muestreo aproximadamente el 5% de toda la varianza registrada por el CDI. Sólo con eso se responde al segundo punto, pero este procedimiento aporta más, estudiando la variabilidad espacial del CDI en la parcela se puede estimar el número y ubicación de muestras foliares necesarias, lo cual optimizaría el muestro y reduciría su coste.

Comprobado que el desarrollo del cultivo es correcto y que existe una estructura espacial se procede al muestreo foliar. En este punto se podrían emplear rangos de suficiencia o relaciones entre nutrientes para su interpretación. Para tratar de superar el tercer punto y dado que el CDI es un buen estimador del rendimiento del cultivo, se optó por estudiar la relación entre el CDI y los diferentes nutrientes, identificando como limitantes aquellos que expliquen parte de la varianza del CDI. Eso significa confiar en que una relación estadística implique una relación causal, por ello es necesario tomar muchas precauciones en ese estudio para obtener un resultado válido. Ese es un punto en común con las otras metodologías para la interpretación de análisis foliares, las cuales han demostrado que no es una debilidad. Una nueva prueba de ello son los resultados obtenidos en ambos campos. En Pacthy se identifica el K, el Ca y el N como deficientes, lo cual es coincidente con lo deducido en el muestreo del suelo y compatible con el diagnóstico DRIS. En el Haj no se identificaron factores limitantes, lo cual volvió a ser coincidente con lo diagnosticado por otros métodos y explica el alto y uniforme rendimiento del cultivo.

Si al llegar la cosecha se realiza un nuevo muestreo, entonces es posible comprobar si existe relación entre el CDI y el rendimiento del cultivo, si no existe esa relación entonces la hipótesis será la de la ocurrencia de alguna incidencia entre el muestreo y la cosecha, la cual podría llegar a identificarse analizando el mapa del CDI y del rendimiento del cultivo de todo el campo obtenido mediante los factores espaciales.

Como se ha comentado anteriormente, en el campo Haj ocurrió una incidencia entre muestreo y cosecha. El alto rendimiento del cultivo coincidía con la alta estimación del mismo obtenida mediante el CDI, pero sus patrones espaciales no coincidían. Comparando los mapas del CDI y del rendimiento del cultivo se observó que las posiciones ideales relativas habían cambiado desde el muestreo a la cosecha

de tal forma que hizo sospechar de una precipitación inusualmente intensa, se consultó el registro meteorológico y se confirmó la incidencia.

The above results are evidence that would be possible to estimate the level of nutrients in the plant quickly, accurately and cheaply. This development alone will not be a great help to the farmers because of the lack of a methodology for efficient interpretation of the levels of nutrients in the plant.

It is possible to make a detailed estimate of the level of nutrients in an agricultural field (radiometry, leaf analysis or other methods) and that this does not imply an improvement in the crop yield. That could happen for several reasons:

- 1. Because it is a bad year in which the best option is to opt for an agricultural management of minimum cost. The crop sampling has to be canceled because it would not be profitable. It is necessary to estimate this circumstance at the time of sampling.
- 2. Because there is not spatial structure in the crop development. The sampling points are not good estimators of their neighborhood and therefore the recommendations in unsampled points (interpolations) would be wrong, ruining the potential improvement. This should be investigated before wasting resources on a crop sampling. It could be necessary to use zoning techniques to delineate areas of management.
- 3. Because the rules for the interpretation of the levels of nutrients (sufficiency ranges or relationships between nutrients) are not specific of the crop geographical area and therefore they are not effective. Different studies showed the limited generalizability.
- 4. Because some event occurs between the sampling of the crop and the harvest, which adversely affects the crop yield. In that case the event should be identified to increase the knowledge and be able to avoid it in the future.

The results shown in the fourth article included in this thesis answer all the above questions.

The crop development index (CDI) showed gather more information about the state of the crop than the height or the Nester independently. It turned out to be a good estimator of the spatial variability of the crop in both fields and in the field Pacthy it was good estimator of crop yield. The CDI was not good estimator of production in Haj because between sampling and harvest rained 228mm above the mean, incident that affected the development of the crop. Known this it became clear that the CDI is an efficient estimator of crop yield. Viability thresholds that determine when the intervention in the field is cost-effective could be identified, which responds to the first point of the above.

The relationship between the CDI and the spatial factors (surface functions and topographic variables) was studied to check the spatial structure, responsible for representing the factors that could cause the spatial variability. Spatial structure was found in the two fields, attributing to chance and sampling error only the 5% of the variance recorded by CDI. That answers the second point, but this procedure provides more. The number and location of necessary samples can be estimated studying the spatial variability of the CDI in the field, it would optimize the sampling and reduce its cost.

Only if the crop development is correct and there is a spatial structure, leaf sampling is carried out. At this point one could use sufficiency ranges or relationships between nutrients for its interpretation, but in order to overcome the third point and since the CDI is a good estimator of crop yield, we decided

to study the relationship between the CDI and the different nutrients, identifying as limiting to those that explain part of the variance of the CDI. That means trusting that a statistical relationship implies a causal relationship. It is necessary to take great care in this study to obtain a valid result. That is a point in common with the other methodologies for interpreting leaf analysis, which have shown that it is a valid hypothesis. New proofs of it are the results in both fields. It identifies the K, Ca and N as deficient in Pacthy, which is coincident with the inferred from the soil sampling and supported by DRIS. In Haj the limiting factors were not identified, which was again coincident with other methods and it explains the high and uniform crop yield.

If at harvest a new sampling is carried out, then it is possible to check the correlation between the CDI and the crop yield. If there is not relationship, then the hypothesis would be the occurrence of any incident between sampling and harvest, which could be identified by analyzing the map of CDI and crop yield obtained by spatial factors.

As mentioned above, in the field Haj an incidence occurred between sampling and harvest. The high crop yield coincided with the high estimate obtained by the CDI, but their spatial patterns differed. Comparing CDI maps and crop yield was observed that the ideal positions (relative) had changed from sampling to harvest. This made us suspicious of precipitation; an unusually intense precipitation could explain the observed. The meteorological record was consulted and the incident was confirmed.

Novedades introducidas / Innovations introduced

Estudio radiométrico:

- El empleo de una combinación de técnicas de la minería de datos rigurosamente evaluadas mediante repeticiones de la validación cruzada.
- La búsqueda de modelos con mayor capacidad de generalización. Pese a los evidentes cambios durante el desarrollo del cultivo, se buscaron rasgos espectrales relacionados estrecha y firmemente con el nivel de nitrógeno en planta, los cuales fueron encontrados.

Diagnóstico agronómico:

- La definición de un índice de desarrollo del cultivo que sirve para estimar el rendimiento del cultivo, como referencia con la que comparar las concentraciones de los nutrientes, etc.
- El estudio de la variabilidad espacial para determinar la conveniencia de adoptar la agricultura de precisión, la necesidad de emplear técnicas avanzadas para la delimitación de zonas de gestión, etc.
- La realización de un diagnóstico agronómico basado en evidencias obtenidas en el mismo campo y su evaluación al final de la campaña.
- ...

Radiometric research:

- The use of a combination of data mining techniques rigorously evaluated by cross validation.
- The search for models with higher generalization ability. Despite the obvious changes during the crop development, we sought spectral features closely and firmly related to the level of nitrogen in plant.

Agronomic diagnosis:

- The definition of a crop development index used to estimate the crop yield. It also serves as a reference with which to compare the concentrations of nutrients, etc.
- The study of the spatial variability to determine the advisability of adopting precision agriculture, the need to employ advanced techniques for the delimitation of the agricultural management zones, etc.
- Performing an agronomic diagnosis based on evidence obtained in the same field and its assessment at the end of the campaign.
- ...

Líneas de trabajo futuras / Future research

Estudio radiométrico:

- Identificar la magnitud de la calibración necesaria para ajustar los modelos radiométricos a las condiciones específicas de cada campaña. Determinar si las longitudes de onda son válidas y sólo hay que modificar los umbrales del árbol de decisión.
- Tratar de reproducir los resultados obtenidos en el estudio radiométrico empleando medidas de la reflectancia del dosel de vegetación en lugar de la firma espectral de las hojas. Ello supondría un logro rápidamente transferible al sector. Si eso es posible entonces se puede desarrollar un sistema montado en maquinaría agrícola que en tiempo real estime el estado nutricional del cultivo. Dada la agilidad del sistema podría barrer grandes superficies en poco tiempo, esto haría rentable la inversión en agricultura de precisión.

Diagnóstico agronómico:

- Explorar nuevas formulaciones del índice de desarrollo del cultivo (CDI). Determinar si medidas radiométricas y/o descriptores del patrón de desarrollo colonial del cultivo pueden mejorar la eficacia del CDI.
- Comprobar la idoneidad del CDI para diferentes cultivares (trigo de invierno) y otros cereales, incluso para otros cultivos.
- Realizar estudios que determinen umbrales para la media y la desviación del CDI, los cuales ayuden en la toma de decisiones del agricultor.
- Comprobar si las interpolaciones empleando los factores espaciales pueden mejorar incluyendo imágenes remotas de toda la parcela.

• Continuar con los ensayos de la metodología, tratando de buscar los escenarios más complejos, para determinar su potencial.

Radiometric research:

- Identifying the magnitude of the necessary calibration to adjust the radiometric models to the specific conditions of each campaign. Determine if the wavelengths are valid and it just needs to modify the thresholds of the decision tree.
- Trying to reproduce the results obtained in the study using canopy reflectance instead of the spectral signature of the leaves. It could mean an achievement quickly transferable to the farms. If that is possible then one can develop a system mounted on farm machinery that in real time estimates the nutritional status of the crop. Given the agility of the system, it could sweep large areas in a short time. This would make profitable the investment in precision agriculture.

Agronomic diagnosis:

- Explore new formulations of the crop development index (CDI). Determine whether radiometric measurements and / or the pattern of colonial development can improve the efficiency of the CDI.
- Check the suitability of the CDI for different cultivars (winter wheat) and other cereals, even for other crops.
- Studies to determine thresholds for the mean and the standard deviation of the CDI, which help in the decision making of the farmer.
- Check if interpolations using spatial factors along with remote images can achieve better results.
- Continue testing the methodology, trying to look for the more complex scenarios, to determine its potential.

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Conclusions / Conclusions

En la firma espectral del cultivo existen rasgos relacionados con el nivel de nitrógeno en planta, los cuales permanecen estables durante un amplio intervalo fenológico.

Aún en un amplio rango de condiciones de desarrollo, es posible desarrollar modelos radiométricos eficaces, pero se desconoce si han de ser calibrados cada campaña y si sería posible ajustarlos para operar con medidas de reflectancia del dosel de vegetación.

La metodología SIOPP ha probado ser eficaz realizando el diagnóstico agronómico de dos explotaciones agrícolas reales en las que los problemas eran complejos. Con las evidencias disponibles y dado el bajo coste añadido que implica su implementación, ya se considera una alternativa al uso de rangos de suficiencia o relaciones entre nutrientes para la interpretación de los análisis foliares.

Cuando no existan zonas en el campo con un buen desarrollo del cultivo, zonas de referencia, SIOPP no podrá realizar el diagnóstico. Las condiciones de desarrollo del cultivo han de estar alejadas del óptimo, esa primera corrección, obvia revisando un tratado de agronomía, es un requisito de la metodología en casos extremos.

En caso de existir severa heterogeneidad (márgenes abruptos) o si hay que diagnosticar plantaciones con centenares de hectáreas de extensión, SIOPP puede presentar problemas ante la debilidad de modelar barreras y/o infinidad de gradientes. En ese caso sería necesario realizar un estudio previo para la delimitación de las zonas de gestión, esta es una de las líneas de trabajo futuras.

There are features in the spectral signature of the crop related to plant nitrogen (N) content, which remain stable over a wide range of phenological stages.

Even in a wide range of development conditions, it is possible to develop effective radiometric models, but it is unknown if they have to be calibrated in each campaign and whether it would be possible to adjust them to operate with measures of vegetation canopy reflectance.

The spatial interpretation of plant parameters (SIOPP) has proven to be effective for the agronomic diagnosis of two real farms where the problems were complex. With the available evidence and given the low added cost involved in its implementation, it is considered as an alternative to using sufficiency ranges and relationships between nutrients for interpreting leaf analysis.

When there are not areas in the field with a good crop development, reference areas, SIOPP cannot make the diagnosis. The conditions for crop development should be away from the optimum. That first correction, which has to be obvious after reviewing any textbook of agronomy, is a requirement of the methodology in extreme cases.

In case of severe heterogeneity (abrupt margins) or if it has to diagnose plantations with hundreds of hectares, SIOPP can present problems because of the difficulty of modeling steep barriers and / or countless gradients. In that case it would be necessary to carry out a study for the definition of areas of management; this is one of the future lines of work.