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Optimizing N-fertilization decisions of wheat and maize by advanced soil- and plant analysis

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List of abbreviations

BNF	Biological nitrogen fixation
C	Carbon
$CaCl_2$	Calcium chloride
cm, cm^3	Centimeter, cubic centimeter
g	Gram
ha	Hectare
KCl	Potassium chloride
LAI	Leaf area index
M	Molar mass
mm	Amount of precipitation (1 mm ≙ 1 liter/m^2)
m^2	Square meter
N	Nitrogen
N_2	Dinitrogen
NDVI	Normalized difference vegetation index
NDRE	Normalized difference red-edge index
NH_3	Ammonia
NH_4	Ammonium
N_{min}	Soil mineral nitrogen (nitrate-N + ammonium-N)
NNI	Nitrogen nutrition index
NO	Nitric oxide
NO_2	Nitrogen dioxide
NO_3^-	Nitrate anion
NO_x	Nitrogen oxides
N_2O	Nitrous oxide
HNO_3	Nitric acid
HONO	Nitrous acid
NUE	Nitrogen use efficiency
PAN	Peroxyacyl nitrates
REIP	Red-edge inflection point
Tg	Teragram (≙ 10^9 kilograms)

Summary

Nitrogen (N) is an essential plant nutrient with significant functions concerning plant metabolism. Among all essential macronutrients, N is quantitatively the most important. Although nitrogen is abundant in the atmosphere (N_2), the availability of this source of nitrogen for many crops is not given. The uptake of N from agricultural soils is also limited for plants because only a small portion of nitrogen is present in the soil in a form available for plant uptake. These conditions justify the frequent use of N-fertilizers in agriculture, which also usually increase the yield and quality of crop products. However, crops in general, as well as globally important crops such as wheat (*Triticum aestivum* L.) and maize (*Zea mays* L.) in particular, only partially use the N of the applied fertilizer. Thus, nitrogen from N-fertilizers not only accumulates in the harvest products but also enters the environment. Nitrogen affecting the environment can cause considerable damage, e.g., in the form of nitrate (NO_3), ammonia (NH_3) and nitrous oxide (N_2O). Therefore, all stakeholders in agriculture strive to avoid nitrogen losses or increase N use efficiency, which can be done through multiple measures.

To estimate the nitrogen requirement of crops at the beginning of vegetation, the examination of the mineral nitrogen content of the soil through the N_{min} method (nitrate-N + ammonium-N, "N_{min}") is widely used. However, sampling and analysis are time-consuming, labor-intensive, and costly. During the growing season, optical detection of the canopy reflectance signature is a long-established method to estimate the nitrogen nutritional status of the crop. The reflectance signature is typical for plants and differs depending on the N-supply. Several different spectral sensors and carrier vehicles are available for reflectance measurements. The advantage of this method is the fast, non-destructive and cost-efficient application. However, methodological error limits that take agronomic aspects into account are still lacking.

Therefore, this work, including three chapters, aims, (i) to optimize sampling per field for N_{min} analysis and therefore make it more practicable (chapter *I*) and, (ii) to develop agronomically-based error limits for the spectral detection of N uptake in wheat (chapter *II*) and nitrogen-related traits and grain yield in maize (chapter *III*).

Chapter *I* includes the sampling of twelve fields for N_{min} at the beginning of vegetation at different locations within two years. Field sampling were usually done in a grid pattern and at each sampling point in 30 cm increments down to 60 or 90 cm. Sampling was carried out both with a set of two gauge augers (Pürckhauer) and with a soil sampling device mounted on a tractor. The further sample processing as well as the analysis complied with the common regulations for N_{min} samples. In a further step, the results of the N_{min} sampling were compared with reflectance data from satellite measurements (Sentinel-2). Nitrogen fertilization field experiments included three one-year trials in

wheat (chapter *II*) and one two-year trial in maize (chapter *III*). The field trials include the harvest of plant samples during the growing season with further analysis of the nitrogen content and the dry matter as well as the grain yield at harvest (exclusively chapter *III*). Further N-related traits were calculated. Destructive sampling and spectral measurements with different sensors were carried out simultaneously. Afterward, the reflectance data were calculated as spectral indices. In a further step, the spectral assessment of the N uptake of wheat and N-related traits and grain yield of maize were analyzed.

Chapter *I* reports the possibility to sample wheat and maize fields for mineral nitrogen in the soil (nitrate-N + ammonium-N, "N_{min}") with only two samplings per field. This result is valid with a maximum error of ±10 kg nitrate-N ha^{-1}, which, however, can be regarded as acceptable and practicable in comparison with other sources of error affecting the N_{min}-method. Furthermore, the reduced N_{min} sampling strategy is more precise for the individual field, especially for wheat, than the use of crop-specific, regionally representative N_{min} values offered by the official advisory authorities. These results were obtained for field sizes in the range of 1.0–12.7 ha and have yet to be verified for larger fields. In addition, heterogeneous fields should be sampled site-specific. Moreover, the results suggest that annual N_{min} soil sampling is necessary because it is influenced by yearly differing weather conditions. However, the soil sampling can further be simplified by combining the individual soil layer samples into one composite sample, which accordingly reduces the cost of analysis. The aggregation of single soil layers is more recommended for the determination of the absolute N-fertilization requirement. In the case of no-till managed fields, the individual soil layers should be analyzed separately. During vegetation, spatial variations of crops within a field due to different N_{min} levels could not be detected by multispectral satellite imagery (Sentinel-2), again highlighting the need for soil sampling.

Chapter *II* elaborates on agronomically-based error limits for the spectral detection of N uptake in wheat. Conventional statistics such as the coefficient of determination (R^2) are strongly dependent on the differentiation of the N uptake, which often occurs only at later stages of development (e.g., the influence of N-fertilization on N uptake). RMSE and MAE values have the advantage that the error is given in the unit of the respective target trait. However, since it is only an average value, this indicates that many observations are overestimated or underestimated. The study could determine an agronomic error of ±15 kg N uptake ha^{-1} with a probability of at least 80 %. This interval is valid until BBCH 50. At earlier stages of development, ±10 kg N uptake ha^{-1} may also be sufficient. Aerial- (UAV) and ground-based (Phenotrac IV) systems provided roughly comparable results in spectral detection of N uptake, with spectral indices combining REDEDGE and NIR bands proving advantageous. For

detection of the N uptake in wheat, the differentiation of biomass is more crucial than the differentiation of the N content.

Chapter *III* analyzes agronomically-based error limits of the spectral detection of N-related traits (aboveground and grain N uptake, and NNI) and grain yield in maize. Commonly used statistics such as the coefficient of determination (R^2) are highly dependent on the differentiation of the respective target trait, which often occurs at later stages of development (e.g., the influence of the N-fertilization on target traits). Although RMSE and MAE indicate the error in the same unit of the respective target trait, it remains only an average value, which therefore leads to an over- or underestimation for many observations. This work was able to determine an agronomic error of ±25, ±40 kg N ha^{-1}, ±0.2, and ±1.4 t ha^{-1} for grain and aboveground N uptake, NNI, and grain yield, with a probability of at least 80 %. The error limits are consistent across experimental years and growth stages, as spectral indices were largely dominated by biomass. Across all traits, best-performing indices combine GREEN, REDEDGE, and NIR bands.

The **general discussion** compares and classifies the results of the individual chapters with existing studies. Furthermore, the usefulness of field experiments in agricultural research is discussed. This is based on the fact that findings from controlled (laboratory) experiments can only be transferred to agricultural agroecosystems to a limited extent because a large number of uncontrollable variables influences the treatment effects. Furthermore, future investments in the education of research staff are discussed as equally necessary.

Zusammenfassung

Stickstoff (N) ist ein essentielles Nährelement für die Pflanze mit bedeutenden Funktionen im pflanzlichen Stoffwechsel. Unter allen essentiellen Makronährstoffen hat N quantitativ die größte Bedeutung. Obwohl Stickstoff in der Atmosphäre (N_2) reichlich vorhanden ist, ist für viele Kulturpflanzen die Verfügbarkeit dieser Stickstoffquelle nicht gegeben. Auch die Aufnahme von Stickstoff aus landwirtschaftlich genutzten Böden ist für Pflanzen eingeschränkt, da der Stickstoff nicht in ausreichender Menge in einer für die Pflanzen verfügbaren N-Form vorhanden ist. Diese Gegebenheiten begründen den häufigen Einsatz von N-Düngemitteln in der Landwirtschaft, deren Verwendung in der Regel auch eine Ertrags- und Qualitätssteigernde Wirkung bei den Ernteprodukten bewirkt. Kulturpflanzen im Allgemeinen als auch global bedeutende Kulturen wie z.B. Weizen (*Triticum aestivum* L.) und Mais (*Zea mays* L.) im Speziellen nutzen den eingesetzten N-Dünger allerdings nur teilweise, sodass Stickstoff aus N-Düngemitteln sich nicht nur im Erntegut anreichert, sondern auch in die Umwelt gelangt. Der die Umwelt betreffende Stickstoff kann dort z.B. in Form von Nitrat (NO_3), Ammoniak (NH_3) und Lachgas (N_2O) erhebliche Schäden verursachen. Daher sind alle Akteure in der Landwirtschaft bestrebt, Stickstoffverluste zu vermeiden bzw. die N-Nutzungseffizienz zu erhöhen, was durch eine Fülle an Maßnahmen erfolgen kann.

Um den Stickstoffbedarf der Kulturen zu Vegetationsbeginn abschätzen zu können, ist die Untersuchung des mineralischen Stickstoffgehaltes des Bodens mit der N_{min}-Methode (Nitrat-N + Ammonium-N, “N_{min}”) weit verbreitet. Die Probennahme und die Analytik ist jedoch zeit-, arbeits- und kostenaufwendig. Während der Vegetationsperiode ist die optische Erfassung der Reflexionssignatur des Pflanzenbestandes eine bereits seit Jahren etablierte Möglichkeit den Stickstoffernährungszustand der Kultur abzuschätzen. Die Reflexionssignatur bei Pflanzen zeigt einen typischen Verlauf und differenziert je nach N-Versorgung. Für Reflexionsmessungen stehen eine Reihe an unterschiedlichen Spektralsensoren sowie Trägerfahrzeuge zur Verfügung. Der Vorteil dieser Methode ist die schnelle, zerstörungsfreie und kosteneffiziente Anwendung. Allerdings fehlt es bei der Bewertung dieser Methode bisher an Fehlergrenzen, die agronomische Gesichtspunkte miteinbeziehen.

Daher verfolgt diese aus drei Kapiteln bestehende Arbeit einerseits den Zweck, (i) die N_{min}-Probenahme je Feld zu optimieren und daher anwenderfreundlicher zu gestalten (Kapitel *I*), und andererseits (ii) agronomisch begründete Fehlergrenzen bei der spektralen Erfassung der N-Aufnahme bei Weizen (Kapitel *II*), sowie stickstoffbezogener Merkmale und des Kornertrages bei Mais (Kapitel *III*) zu erarbeiten.

In Kapitel *I* wurden innerhalb von zwei Jahren an unterschiedlichen Standorten zwölf Felder auf N_{min} zu Vegetationsbeginn rasterförmig beprobt. Die Probenahme erfolgte sowohl mit dem Pürckhauer-Bohrstock, als auch mit einem am Traktor montierten Bodenprobenentnahmegerät jeweils in 30 cm Bodenschichten bis maximal 90 cm Bodentiefe. Die weitere Probenverarbeitung sowie die Analyse entsprachen den gängigen Vorschriften für N_{min}-Proben. Die Ergebnisse der N_{min}-Beprobung wurden in einem weiteren Schritt mit Reflexionsdaten aus Satellitenmessungen (Sentinel-2) verglichen. In Kapitel *II* wurden im Feld drei einjährige Stickstoffsteigerungsversuche bei Winterweizen, sowie in Kapitel *III* ein zweijähriger Stickstoffsteigerungsversuch bei Mais durchgeführt. In den Feldversuchen wurden während der Vegetationsperiode Pflanzenproben entnommen und der Stickstoffgehalt und die Trockenmasse analysiert sowie der Kornertrag (ausschließlich Kapitel *III)* erfasst. Weitere Merkmale wurden berechnet. Zeitlich abgestimmt mit den destruktiven Beprobungen wurden Spektralmessungen mit unterschiedlichen Sensoren durchgeführt und anschließend die Reflexionsdaten zu Spektralindizes verrechnet. Die spektrale Erfassung der N-Aufnahme bei Weizen sowie der stickstoffbezogenen Merkmale und des Kornertrages bei Mais wurde analysiert.

Kapitel *I* zeigt auf, dass landwirtschaftlich genutzte Felder mit nur zwei Probenahmestellen (Einstichen) je Feld auf mineralischen Stickstoff im Boden (Nitrat-N + Ammonium-N, "N_{min}") beprobt werden können. Die Reduzierung der Probenahmestellen beinhaltet einen maximalen Fehler von ±10 kg Nitrat-N ha^{-1}, der im Vergleich zu anderen die Methode betreffenden Fehlerquellen jedoch als akzeptabel und praxistauglich angesehen werden kann. Die reduzierte N_{min}-Beprobungsstrategie ist darüber hinaus für das einzelne Feld, insbesondere bei Weizen, repräsentativer als die Verwendung von überregionalen N_{min}-Werten aus der Offizialberatung. Diese Ergebnisse wurden für Feldgrößen im Bereich von 1.0–12.7 ha ermittelt und sind für größere Felder noch zu prüfen. Außerdem sollten heterogene Felder teilflächenspezifisch beprobt werden. Weiterhin konnte festgestellt werden, dass eine jährliche N_{min}-Bodenuntersuchung nötig ist, da Wetterbedingungen den Gehalt an mineralischem Bodenstickstoff beeinflussen. Diese kann jedoch vereinfacht werden, indem die Proben der verschiedenen Bodenschichten zu einer Mischprobe vereint werden, was dementsprechend die Analysekosten reduziert. Die Zusammenlegung der Bodenschichten wird im Besonderen für die Düngebedarfsermittlung empfohlen. Für Felder, die in Direktsaat bewirtschaftet werden, sollten die einzelnen Bodenschichten getrennt analysiert werden. Während der Vegetation konnten Variationen im Pflanzenbestand aufgrund unterschiedlicher N_{min}-Gehalte nicht durch multispektrale Satellitenbilder (Sentinel-2) nachgewiesen werden, was wiederum die Notwendigkeit von Bodenuntersuchungen verdeutlicht.

Kapitel *II* erarbeitet agronomisch begründete Fehlergrenzen für die spektrale Erfassung der N-Aufnahme bei Weizen. Herkömmliche statistische Gütemaße wie das Bestimmtheitsmaß (R^2) sind stark von der Differenzierung der N-Aufnahme abhängig, was häufig erst in späteren Entwicklungsstadien auftritt (z.B. Einfluss der N-Düngung auf die N-Aufnahme). RMSE und MAE haben zwar den Vorteil, dass der Fehler in der Einheit des jeweiligen Zielmerkmales angegeben wird, allerdings ist dies nur ein Mittelwert. Viele Beobachtungen werden dadurch über- oder unterschätzt. Die Arbeit konnte einen agronomischen Fehler von ±15 kg N-Aufnahme ha^{-1} bei einer Wahrscheinlichkeit von mindestens 80% ermitteln. Dieses Intervall ist gültig bis BBCH 50. In früheren Entwicklungsstadien können auch ±10 kg N-Aufnahme ha^{-1} ausreichend sein. Das luftgestützte (UAV) und das bodenbasierte (Phenotrac IV) System lieferten in etwa vergleichbare Ergebnisse bei der spektralen Erfassung der N-Aufnahme, wobei spektrale Indizes, die die Banden REDEDGE und NIR kombinierten am besten geeignet waren. Für die Erfassung der N-Aufnahme bei Weizen ist die Differenzierung der Biomasse entscheidender als die des N-Gehaltes.

Kapitel *III* analysiert agronomisch begründeten Fehlergrenzen der spektralen Erfassung von stickstoffbezogenen Merkmalen (N-Aufnahme der Biomasse und des Korns, NNI) und des Kornertrages bei Mais. Häufig verwendete statistische Gütemaße wie das Bestimmtheitsmaß (R^2) sind stark von der Differenzierung des jeweiligen Zielmerkmals abhängig, was häufig erst in späteren Entwicklungsstadien auftritt (z.B. Einfluss der N-Düngung auf die Zielmerkmale). RMSE und MAE geben den Fehler zwar in der Einheit des jeweiligen Zielmerkmales an, jedoch nur als gemittelten Fehler, was für viele Beobachtungen deshalb zu einer Über- oder Unterschätzung führt. Die Arbeit konnte einen agronomischen Fehler von ±25, ±40 kg N ha^{-1}, ±0.2, und ±1.4 t ha^{-1} für die Korn und oberirdische N-Aufnahme, den NNI und den Kornertrag bei einer Wahrscheinlichkeit von mindestens 80% ermitteln. Die Intervallgrenzen waren über die Versuchsjahre und Wachstumsstadien hinweg konsistent, da die spektralen Indizes weitestgehend von der Biomasse dominiert werden. Alle Zielmerkmale konnten am besten erfasst werden, wenn die spektralen Indizes die Banden GREEN, REDEDGE und NIR kombinierten.

In der **übergeordneten Diskussion** werden die Ergebnisse der einzelnen Kapitel mit bereits existierenden Studien verglichen und eingeordnet. Darüber hinaus wird die Nützlichkeit von Feldexperimenten in der Agrarforschung diskutiert. Dies beruht auf der Gegebenheit, dass Erkenntnisse aus kontrollierten (Labor-) Versuchen nur eingeschränkt auf landwirtschaftliche Agrarökosysteme übertragen werden können da die Behandlungseffekte durch eine Vielzahl von unkontrollierbaren Variablen beeinflusst werden. Darüber hinaus werden zukünftige Investitionen in die Ausbildung des Forschungspersonals als ebenso notwendig diskutiert.

1 General introduction

1.1 Nitrogen: current and future agricultural challenges

In the 21st century, agriculture and food systems are facing the challenge of meeting the needs of a growing world population (VOS AND BELLÙ, 2019). GERLAND ET AL. (2014) expect a world population of 9.6 billion in 2050 and 10.9 billion in 2100. In addition, it is estimated that global crop demand will have increased by 100 % in 2050 compared to 2005 (TILMANN ET AL., 2011). Although agricultural production tripled between 1960 and 2012, conditions have changed and future challenges are becoming more prevalent such as the limited expansion of arable land and water resources as well as climate change and loss of biodiversity (NORRIS 2008; LOBELL ET AL., 2011; ASSENG ET AL., 2015; DUDLEY AND ALEXANDER, 2017; PEREIRA 2017; VOS AND BELLÙ, 2019). Additionally, sustainable agriculture is targeted (REGANOLD ET AL., 1990; VELTEN ET AL., 2015). *Figure 1* illustrates the relationships.

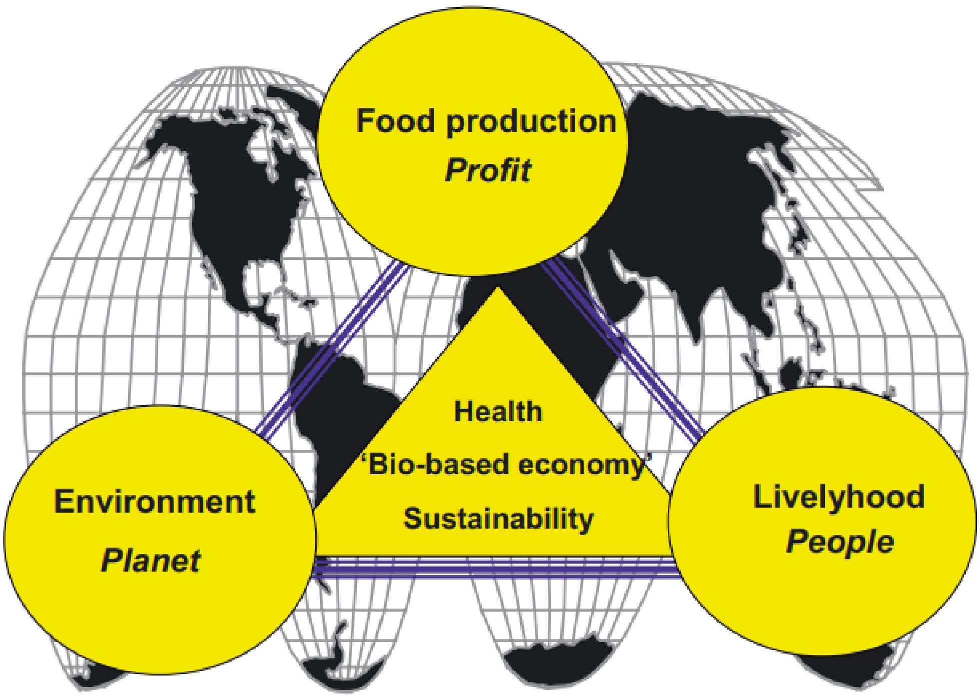

Figure 1: Sustainable agriculture presented as a conceptual 3-P framework: People-Planet-Profit (SPIERTZ, 2009).

ROCKSTRÖM ET AL. (2009) identified boundaries for nine earth-system processes, which, if crossed, could generate unacceptable environmental changes. Besides climate change and the loss of biodiversity, the nitrogen cycle has already transgressed its boundary, which could potentially harm human development. The worldwide nitrogen (N) cycle is mainly influenced by the Haber-Bosch process (*Figure 2*), where ammonia, a chemically reactive highly usable form of N can be synthesized by reacting hydrogen with atmospheric dinitrogen in the presence of iron at high temperatures and pressures. According to estimates, the lives of around half of humanity in 2008 are made possible due to the Haber-Bosch nitrogen (ERISMAN ET AL., 2008).

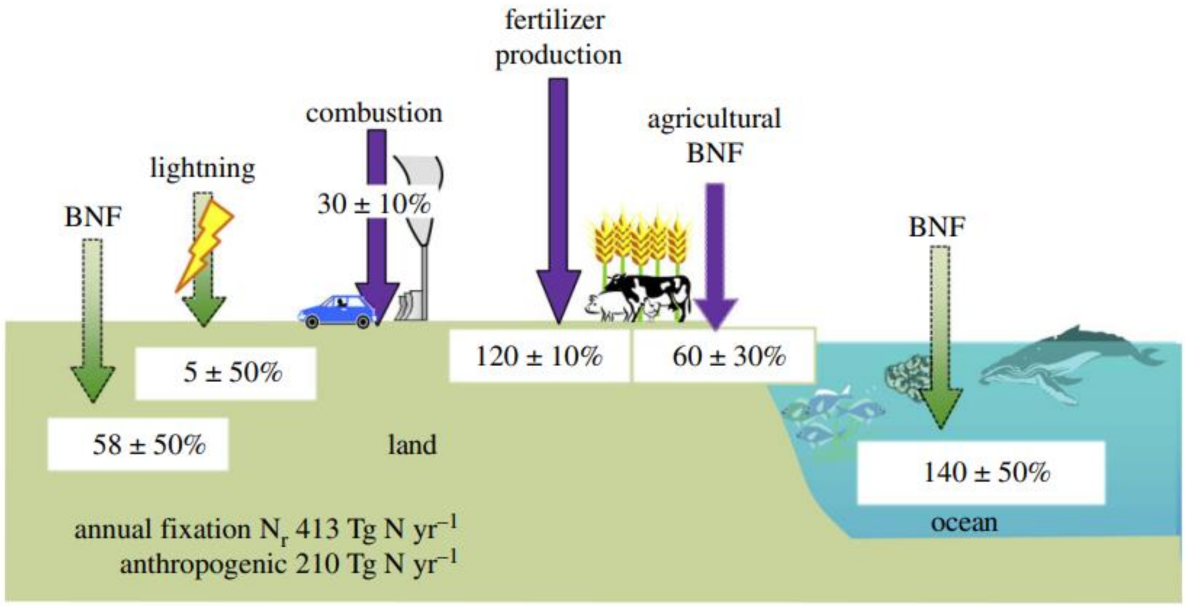

Figure 2: Components of global reactive nitrogen (including NH_3, NH_4, NO, NO_2, HNO_3, N_2O, HONO, PAN, and other organic N compounds) production for 2010. The arrows indicate a transfer from the atmospheric N_2 reservoir to marine and terrestrial ecosystems, where purple and green arrows represent anthropogenic and natural sources. BNF = biological nitrogen fixation (FOWLER ET AL., 2013).

Overall, the natural terrestrial sources of reactive N (63 Tg N year^{-1}) are only half of the fixed N through the Haber-Bosch process in 2010 (120 Tg N year^{-1}) (FOWLER ET AL., 2013). However, a drastic increase in ammonia production leads to a cascade of environmental changes, including water and air pollution, the perturbation of greenhouse-gas levels, and the loss of biodiversity (ERISMAN ET AL., 2007). Nevertheless, access to commercial fertilizers varies widely around the world. In industrialized nations, this has been happening since at least the middle 1900s, whereas large areas of Africa and smaller regions of Latin America and Asia continue to lack access to affordable nitrogen fertilizers (HOULTON ET AL., 2019). To date, recent reports indicate that the consumption of inorganic N-fertilizer in the European Union (EU, 28 countries) increased in recent years and reached 11.6 million tons in 2017 (EUROSTAT, 2022), whereas in Germany, domestic sales of inorganic N-fertilizer have been declining in the last years, reaching 1.265 million tons in the 2020/21 marketing year (STATISTISCHES BUNDESAMT, 2021). Besides the influence of the Haber-Bosch process on the global nitrogen cycle, the worldwide trade of food and feed products plays an important role in the transfer of N (LASSALETTA ET AL., 2014).

Grain cereals contribute strongly to a healthy human diet (BORNEO AND LEÓN, 2011), including the main cereals wheat (*Triticum aestivum* L.), maize (*Zea mays* L.), and rice (*Oryza sativa* L.) (NEUMANN ET AL., 2010; Awika 2011; Sarwar et al., 2013; Ranum et al., 2014), which supply more than half of the calories consumed by humans along with sugarcane and barley (Ross-Ibarra et al., 2007). Global wheat production was 761 million tons in 2020, produced mainly in Asia (45.7%), and Europe (33.5%) (FAOSTAT, 2022). In 2020, Germany harvested 22.2 million tons of wheat in an area of 2.84 million hectares, resulting in an average yield of 7.8 tons per hectare (Statistisches Bundesamt, 2022).

Global maize production was 1162 million tons in 2020, produced mainly in America (50.1%), Asia (31.4%), and Europe (10.7%) (FAOSTAT, 2022). In 2020, Germany harvested 4.0 million tons of grain maize (including corn-cob-mix) in an area of 0.42 million hectares, resulting in an average yield of 9.6 tons per hectare (Statistisches Bundesamt, 2022). For maize, a recent study show possible global changes. Thus, Erenstein et al. (2021) pointed out that one-third of the farms cultivated maize in 2020 with a future 5% increase by 2030, resulting in maize overtaking wheat in terms of the growing area.

1.2 Nitrogen use efficiency as a key to mitigating nitrogen losses

The avoidance of an excessive or deficient supply of N to crops is the key to optimizing trade-offs between yield, profit, and environmental protection. To meet this challenge, an understanding of nitrogen use efficiency (NUE) is needed (Cassman et al., 2002). Many agronomic indices of NUE exist, but in simple terms, NUE is defined as grain production per unit of available N in the soil (Moll et al., 1982; Dobermann, 2005; Udvardi et al., 2021). Globally, the NUE of wheat and maize levels are only at 42% and 46%, respectively (Zhang et al., 2015a). Many tools are available to improve the NUE of crops and to avoid nitrogen losses, including the adaption of source, method, rate, and timing of N-application, the use of nitrogen efficient species and genotypes as well as the control of biotic pests, cover crops, crop rotation, crop residue management, remediation of soil acidity, tillage system, water management, use of animal and green manure, and controlled release of nitrogen through urease- and nitrification inhibitors (Fageria and Baligar, 2005; Noor, 2017). Especially in terms of plant nutrition, further nutrient demand, e.g., potassium and phosphorus, should also be considered (Duan et al., 2014; Salim and Raza, 2020). Additionally, enhancing NUE is only one of four major tools to reduce N losses to the environment. A dietary shift toward more plant-based foods in high-income countries, reduced biofuel production from human-edible foods, and a decrease in food loss and waste should be further considered (Bodirsky et al., 2014; Cassman and Grassini, 2020; Udvardi et al., 2021).

1.3 N-fertilization in cropping systems

The growth of higher plants requires the presence of essential elements. The term essential is defined through three criteria: (i) a plant is unable to complete its lifecycle in the absence of the element, (ii) the function of the element is not replaceable by another element, and (iii) the element is directly involved in plant metabolism. Essential elements, which are present in relatively high concentrations in plants, are called macronutrients and the element nitrogen has on average the highest concentration in the plant shoot dry matter (WHITE AND BROWN, 2010; KIRKBY, 2012). N is most abundant in the atmosphere and yet it is most often deficient in agricultural soils. This paradox exists because the plants require this nutrient element in the largest quantity but only a small proportion of N is present in the soil in a form available to plant uptake (GODWIN AND SINGH, 1998). Therefore, crop production is often limited by N and additional N-fertilization will have to be mostly applied (LADHA ET AL., 2005) because important crop traits such as yield and grain quality are primarily influenced by nitrogen (MASON AND D`CROZ-MASON, 2002; ROBERTSON AND VITOUSEK, 2009; CHEN ET AL., 2015; BARMEIER ET AL., 2017a; PREY ET AL., 2019b). The study of ZHANG ET AL. (2021) indicates that long-term optimal N management (neither over- nor undersupply) in wheat production reduces harm to the ecosystem and human health and increases ecosystem economic benefits.

In agroecosystems, N is available in different forms and rates to different organisms, and specific forms are lost by hydrologic and gaseous pathways (*Figure 3*) (ROBERTSON AND VITOUSEK, 2009). Gaseous losses include N_2O which causes greenhouse warming, and NH_3 which leads to a shift in the ecological balances of natural ecosystems. Hydrologic losses include the displacement of N through eroding sediments in surface water influencing aquatic ecosystems and soluble N in runoff or leachate water, e.g., the negative influence on human health through high-nitrate drinking water (FOLLET AND HATFIELD, 2001). Considering mineral N-fertilization, the latest research by HU AND SCHMIDHALTER (2021) pointed out that the addition of urease inhibitors to urea has great potential to mitigate NH_3 losses in the European Union (EU) as well as in the USA, China, and India. Moreover, the use of urea amended with urease inhibitors is well suited to mitigate N_2O losses compared to ammonium nitrate.

Farmers cannot manage all transformations of the N cycle because important biological processes are affected by given soil properties and also driven by field-specific weather events (MORRIS ET AL., 2018). Additionally, the estimation of soil N budgets in cropping systems is complex. Although the inputs of fertilizer N and irrigation water N are mostly well-known, manure N is often roughly known and the symbiotically fixed N can only be crudely estimated. In the case of the outputs, N removed in harvested crops can be easily estimated whereas gaseous losses are not sufficiently known. Furthermore, long-term research is needed to estimate the change in N storage within the system (MEISINGER AND RANDALL, 1991).

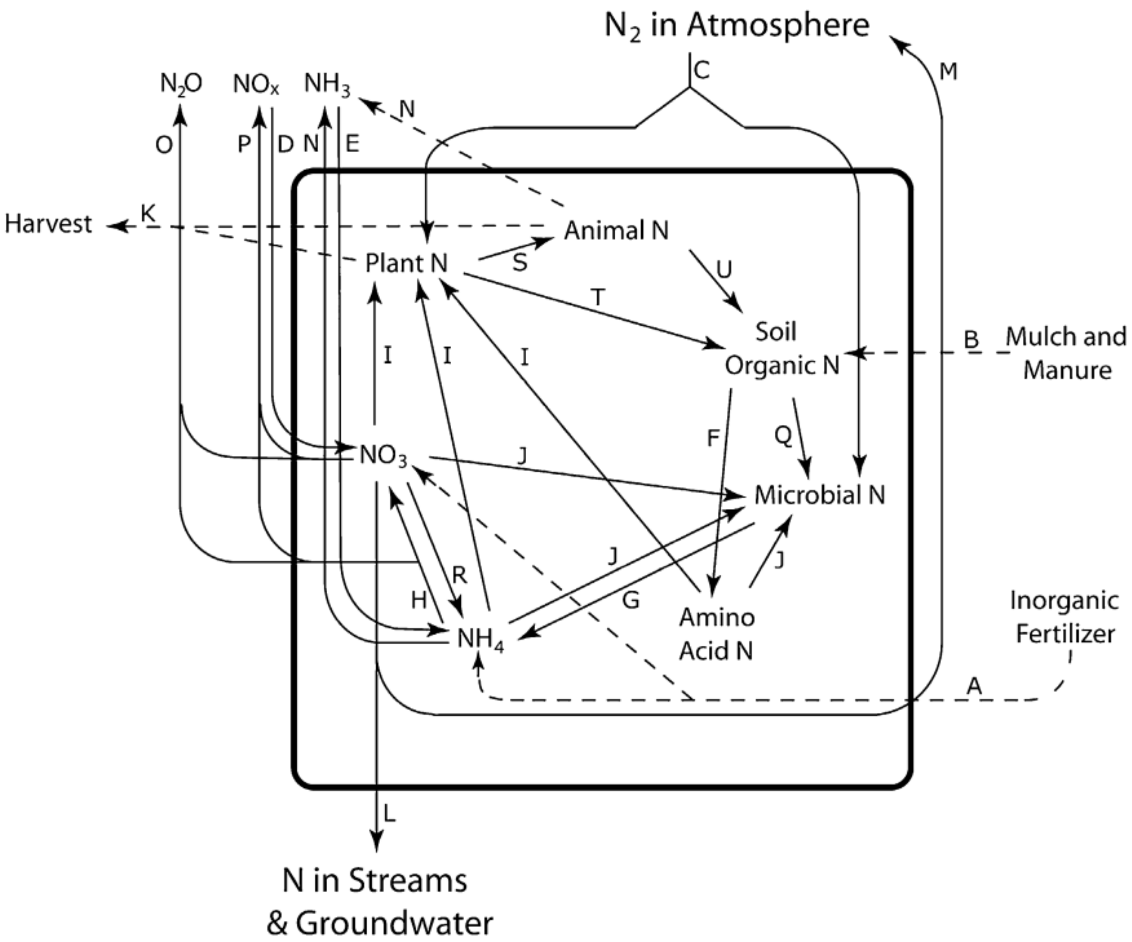

Figure 3: Simplified depiction of pathways of nitrogen (N) in agricultural ecosystems. Transformations of N are shown in solid (occur in all ecosystems) or dashed lines (specific to agricultural systems). A: additions of industrial fertilizer; B: additions of organic N; C: biological N_2 fixation; D: atmospheric deposition of reactive N in oxidized forms; E: atmospheric deposition of ammonia (NH_3) and ammonium (NH_4); F: mineralization of organic N via mobilization of amino acids through the action of extracellular enzymes; G: mineralization of organic N via release of ammonium by microbes; H: nitrification of ammonium; I: plant uptake; J: microbial immobilization; K: losses of N in harvested products; L: losses of N in solution to stream water and groundwater; M: denitrification to dinitrogen; N: NH_3 volatilization from field and animal production; O: losses of nitrous oxide (N_2O); P: losses of reactive oxidized N; Q: uptake of organic N by microbes during decomposition; R: dissimilatory reduction of nitrate to ammonium; S: consumption of plant N by animals; T: flux of N to soil in plant litter; U: flux on N to soil from excretion or animal depth (ROBERTSON AND VITOUSEK, 2009).

1.3.1 N-fertilization of wheat (*Triticum aestivum* L.)

The main aspect to determine the required amount of N-fertilizer is the expected grain yield (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2018b), which can vary greatly between years (LÓPEZ-BELLIDO ET AL., 2005). In Germany, typical winter wheat grain yield expectations (quality level A) of 7–10 to ha^{-1} (14 % water content) need an N supply of 215–250 kg N ha^{-1} (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2018b). Because many factors contribute to the N supply of wheat such as soil properties as well as the past and current management (PETERSEN ET AL., 2012), further factors must be considered such as the soil mineral N (N_{min}), previous organic N-fertilization, consideration of different soils, and pre-crops (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2018b). Nitrogen dressing should follow the nitrogen demand of wheat during growth and development and can therefore vary in terms of the absolute rate, splitting and application time. N-fertilization of wheat aims to enhance (i) tiller formation and spikelet initiation, (ii) ear number, (iii) numbers of fertile spikelets, grains per fertile spikelet and grains per ear, (iv) single grain weight, and (v) protein content (DARWINKEL, 1983; ZÖRB ET AL., 2018). Especially in Western Europe, the absolute amount of N is typically split into three dressings, which are applied approximately at tillering, at the beginning and the end of stem elongation (SWARBRECK ET AL., 2019). The N sources nitrate, ammonium, and urea are equally well suited for the N-fertilization of wheat (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2021A) although yield losses of urea may occur especially on alkaline soils due to ammonia losses if no precipitation follows application (KATYAL ET AL., 1987). Organic fertilizers are also applied to wheat. However, the effect of nitrogen from organic fertilizers in the year of application is low and totals about 35–40 % of mineral-fertilizer equivalents for cattle slurry (GUTSER ET AL., 2005; BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2021B). Although nitrogen promotes the growth of wheat, an excessive supply should be avoided. High N supply increases the length of the lowest internodes and is conducive to lodging, possibly causing grain yield and quality losses (PINTHUS, 1974).

1.3.2 N-fertilization of maize (*Zea mays* L.)

The determination of the absolute amount of the N-fertilization of maize is done similar to wheat taking into account the expected grain yield. Challenges also arise from highly variable yields over the years (BERENGUER ET AL., 2009). In Germany, typical maize grain yield expectations of 8–12 to ha^{-1} (14 % water content) need a N supply of 190–230 kg N ha^{-1} (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2018b). Maize needs a high supply of nutrients, especially in the topsoil, to promote the growth early in the season. This results from very slow plant development and low rooting depth. Due to the good stability of the stem, maize reacts in a not visibly detrimental way to excessive N-fertilization (STURM ET AL., 1994).

In Europe, mineral N-fertilization is often made through band application at planting or broadcast application during early leaf development (up to the seven-leave stage). A combination of both application techniques is also common. Unlike wheat, fertilizer can only be applied at the beginning of maize growth due to the low clearance of tractors and possible etching damage to maize plants. The recovery of different N sources is comparable to wheat. If urea is used before planting, incorporation is favorable although the risk of erosion is to be noted. If urea is used later in the season, precipitation is needed to achieve comparable results as for ammonium nitrate (STURM ET AL., 1994). Similarly to mineral N-fertilizers, organic N-fertilizers are also applied because maize is very effective in using organic fertilizers (DORDAS ET AL., 2008). QUAN ET AL. (2021) emphasized the importance of soil organic C in increasing N use efficiency. However, sufficient N replenishment is not addressed by a high proportion of organic matter in the soil. Although maize shows a considerable N uptake in later stages of development (CIAMPITTI AND VYN, 2011), this can no longer be addressed with the N-fertilization strategy just mentioned.

1.4 N-fertilizer recommendations based on soil- and plant-analysis

The estimate of the absolute amount of N-fertilization based on yield expectation is uncertain because yields can vary greatly between years at one site. Therefore, improved N-fertilizer recommendations are needed, including further methods such as soil- and plant-analysis. Soil analysis refers mainly to assessing soil N mineralization and, regarding this work, the soil mineral N (“N_{min}”, nitrate-N + ammonium-N). Plant analysis encompasses a visual judgment of the crops by growers, destructive plant sampling with a further determination of the total N content, plant-sap/petiole nitrate tests, chlorophyll-meter measurements and, investigated in this work, the use of optical measurements of the crop canopy (remote sensing) to determine N-related traits (DAHNKE AND JOHNSON, 1990; OLFS ET AL., 2005). Although many methods have been developed, SHARMA AND BALI (2017) advocate the combination of two or more methods to optimize nitrogen management.

On-farm methods become increasingly available to help producers to optimize N management decisions because lab-based approaches are often limited under field conditions (FOLLET AND HATFIELD, 2001; OLFS ET AL., 2005). In recent years, a sensor-based approach to detect site-specific yield potential and crop nutrient status is commonly used in agriculture (SCHMIDHALTER ET AL., 2008; MAYFIELD AND TRENGOVE, 2009). Furthermore, approaches with low technical equipment are pursued. RIMPAU (1984) recommended the use of a nitrogen window in grain cereals. This nitrogen window receives 20 to 25 % less nitrogen compared to the common N application rate. During vegetation, this plot indicates a possible nitrogen deficiency earlier than in the rest of the field. The strength and timing of the occurrence of visual differences in the canopy can be used by farmers to decide on further N-applications. A similar approach was successfully carried out by YUE ET AL. (2015) in small-scale wheat fields in China. A precondition for farmers to adopt new techniques is reliability, a minimal additional expense (equipment and time), and easy integration into current operations (FOLLET AND HATFIELD, 2001).

1.4.1 Determination of residual soil nitrogen (N_{min})

Research on the use of N_{min} values to improve N-fertilizer recommendations began several decades ago in several countries. In principle, the soils of fields with higher N_{min} values at the beginning of the vegetation (depending on pre-crop, N leaching over winter, etc.) lead to lower crop response to additional N application and vice versa (OLFS ET AL., 2005). Many sophisticated experiments regarding the framework for soil sampling procedure (DAHIYA ET AL., 1985; BAKER ET AL., 1989; SCHMIDHALTER ET AL. 1991a, 1991b), soil handling and storage (LICKFETT ET AL., 1999) as well as analytical methods (VILSMEIER, 1984) were conducted before N_{min} analysis found its way into agronomic practice. In general, the N_{min} analysis is done by the following procedure: (i) representative soil sampling of the investigated field (15–20 soil cores per ha), (ii) samples taken with an auger from different soil layers (2–3 layers; each 20–30 cm), (iii) homogenizing of the collected soil samples of each soil layer of the field and subsequent use of a subsample, (iv) cooled transport and storage of the soil sample to avoid N mineralization, (v) extraction of the field-moist soil samples with a mild extraction solution (e.g., 1 M KCl, 0.0125 M $CaCl_2$) and further analyzing for nitrate (and ammonium) (HOFFMANN 1991; OLFS ET AL., 2005).

In Germany, N_{min}-based N recommendations were developed by WEHRMANN AND SCHARPF (1979). They found that, on average, N_{min} values in 0–90 cm for loess soils at the beginning of vegetation are 100% plant-available for wheat and thus can be completely included in the calculation of the absolute amount of N-fertilization (approximately 180–200 kg N ha^{-1}). Especially for the first N application early in the season, an “N target value” of 120 kg N ha^{-1} was defined from which the N_{min} value needs to be subtracted to calculate the N-fertilizer rate (OLFS ET AL., 2005).

Nowadays, N_{min} values are used for many crops and different sites and are an integral part of the N-fertilizer recommendations (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2018b). In addition, the individual federal states in Germany can prescribe a mandatory N_{min} soil analysis before the application of significant amounts of nitrogen in areas with high nitrate levels in the groundwater (BLE, 2018). However, there is still a need for optimization, because soil sampling and laboratory analysis are time-consuming and cost-intensive procedure (OLFS ET AL., 2005).

1.4.2 Spectral sensing in agriculture as a tool for plant-analysis

Since the Industrial Revolution, agricultural practices in developed countries have intensified, followed by negative societal and environmental implications. However, the increasing need for food and fiber of a rapidly growing population could be provided. Therefore, Precision Agriculture was developed to ensure safe and sustainable agriculture. Precision Agriculture combines fundamental technologies such as Global Positioning System (GPS), Geographic Information System (GIS), computer modeling, ground-based/airborne/satellite remote sensing, variable rate technology, and advanced information processing for timely in-season and between-season crop management. Therefore, this offers potential benefits in productivity, sustainability, profitability, crop quality, environmental protection, on-farm quality of life, food safety and rural economic development (LIAGHAT AND BALASUNDRAM, 2010). Remote sensing is defined as the measurement and acquisition of information about certain properties of objects, phenomena, or materials by a recording device without physical contact with the features under surveillance (KHORRAM ET AL., 2012). Remote sensing uses methods that measure and detect electromagnetic energy including visible and non-visible radiation that interact with surface materials and the atmosphere (LIAGHAT AND BALASUNDRAM, 2010). In agriculture, the research across a wide range of applications of spectral sensing is under investigation such as weeds (LAMB AND BROWN, 2001; THORP AND TIAN, 2004), plant diseases (ZHANG ET AL., 2019; OERKE, 2020), nutrient monitoring (MAHAJAN ET AL., 2014), crop water stress (ELSAYED ET AL., 2011; BECKER AND SCHMIDHALTER, 2017; GERHARDS ET AL., 2019), and phenotyping (BARMEIER AND SCHMIDHALTER, 2017b; PREY ET AL., 2020). During vegetation, the plant itself is often used as an indicator of N-supply and spectral sensing is a widely used method to detect the N-status of crops, as it is non-destructive and rapid (SCHMIDHALTER ET AL., 2001; OLFS ET AL., 2005; MISTELE AND SCHMIDHALTER, 2008a, 2008b; BARKER AND SAWYER, 2010; WINTERHALTER ET AL., 2011; DIACONO ET AL., 2012; LI ET AL., 2014; CAO ET AL., 2015; ALI ET AL. 2017).

Spectral sensors measure mainly in the wavelength range between 400 and 1000 nm. Vegetation, in particular, shows a typical reflection signature in this spectral range, guided in the visible wavelength range (400–700 nm) by the absorption of pigments (mainly chlorophyll *a* at 430/660 nm and chlorophyll *b* at 450/640 nm as well as other pigments such as xanthophylls and carotenoids at 450 nm) and in the near-infrared (700–1100 nm) by reflection processes in the foliar layers (LILIENTHAL, 2014) (*Figure 4*). Spectral indices can be calculated by using specific wavelengths associated with the N-related traits of maize (MISTELE AND SCHMIDHALTER, 2008a; ZHAO ET AL., 2018; GARCÍA-MARTÍNEZ ET AL., 2020; RAMOS ET AL., 2020) and wheat (MISTELE AND SCHMIDHALTER, 2008b; MISTELE AND SCHMIDHALTER 2010; ERDLE ET AL., 2011; PREY AND SCHMIDHALTER 2019c; DE SOUZA ET AL. 2021).

Spectral measurements can be performed with sensors mounted on carrier vehicles (MISTELE AND SCHMIDHALTER, 2008a; WINTERHALTER ET AL., 2013), handheld sensors (TEAL ET AL., 2006; THOMPSON ET AL., 2015), satellites (KAYAD ET AL., 2019; SKAKUN ET AL., 2021) and unmanned aerial vehicles (UAV) (ZAMAN-ALLAH ET AL. 2015, GNÄDINGER AND SCHMIDHALTER, 2017).

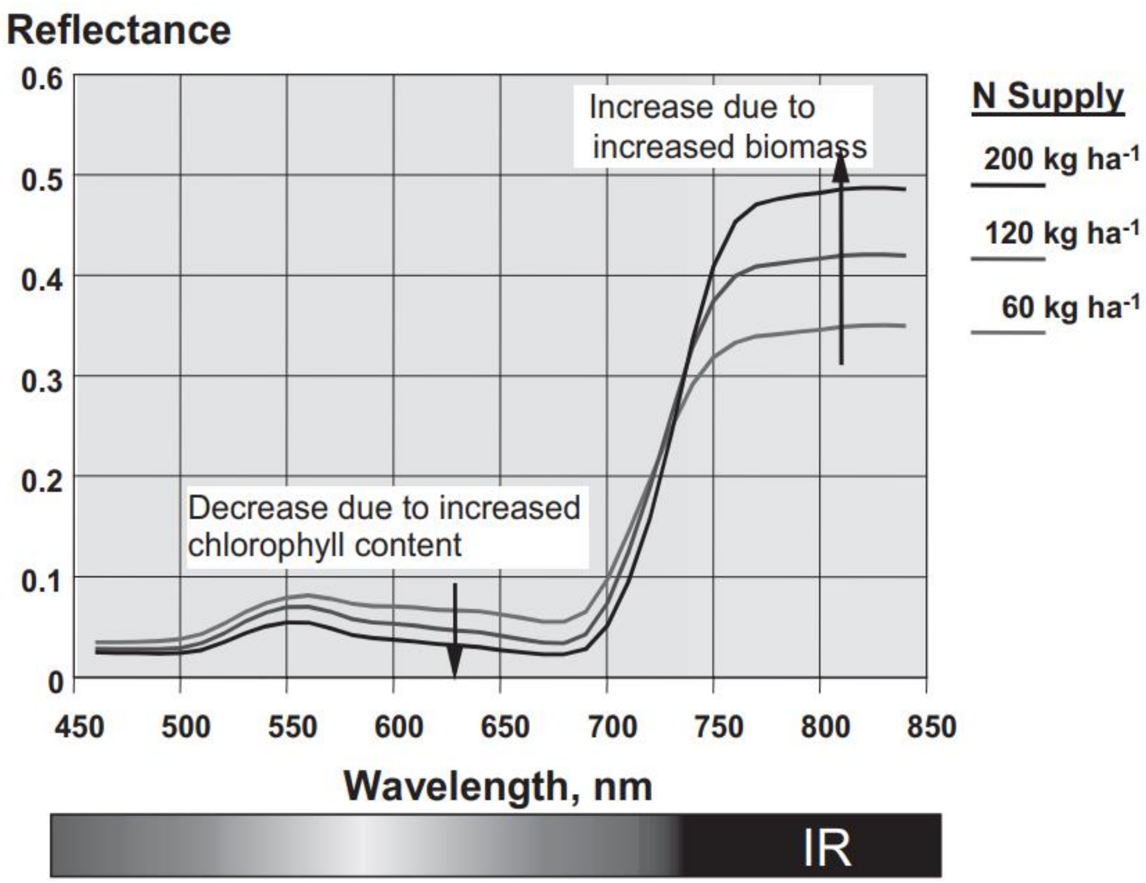

Figure 4: Example of reflectance spectra of winter wheat affected by different N-fertilization. IR refers to the wavelength range of the near-infrared spectrum (OLFS ET AL., 2005).

UAVs have the advantage over ground-based systems that they can capture spatial information simultaneously, enabling measuring without disrupting the surface, and they can generate high-resolution images (AASEN AND BOLTEN, 2018). Especially satellites (i.e., Sentinel-2) promote remote sensing for agricultural applications due to the freely available multispectral data with improved spectral, spatial, and temporal resolution (CLEVERS AND GITELSON, 2013; VIZZARI ET AL., 2019). However, compared to UAVs, one major disadvantage of satellites is the greater ground sample distance (HUNT AND DAUGHTRY, 2018).

Although a wide range of research has been conducted in the field of spectral measurements, to date there is a lack of an agronomically-based evaluation of spectral detection limits of N-related traits of maize and wheat.

2 Thesis objectives and outline

This thesis pursues to optimize the nitrogen fertilization of wheat (*Triticum aestivum* L.) and maize (*Zea mays* L.).

N-fertilizer decisions are based on many assumptions (e.g., grain yield, N-mineralization during the vegetation period) and are further supported by soil- and plant-based measurements. Soil-based measurements include the determination of the residual mineral nitrogen in the soil (nitrate-N + ammonium-N, "N_{min}"). The N_{min}-method is widely used at the beginning of the vegetation in a variety of crops. However, sampling and analysis are time-consuming, labor-intensive and costly, and they need to be further optimized (Section *I*). During vegetation, spectral measurements are commonly used to determine the N uptake and N-related traits of wheat and maize. Many spectral sensors are available to measure the canopy`s reflectance, mounted on various carrier vehicles including aerial- and ground-based systems. However, for in-season N-management decisions, spectral detection limits should be considered. To date, commonly used statistics such as R^2, RMSE, and MAE do not fully attend the agronomic relevance and should therefore be extended including agronomically-based error limits (Sections *II*–*III*).

This thesis is structured cumulatively in three sections.

Section *I* conducted residual mineral soil nitrogen sampling at twelve fields covering many sites in wheat and maize. The aim was to ascertain the necessary sampling intensity (number of samplings per field) to achieve reliable results. Additionally, nitrogen increase experiments in wheat were established to evaluate the usefulness of reduced soil sampling. In a further step, in-season multispectral satellite images (Sentinel-2) were examined to replace the physical soil sampling.

Section *II* defines agronomically-based error limits for the spectral detection of the N uptake in wheat based on data sets including several sites, years, varieties, and growth stages. Additionally, a comparison of aerial- (UAV) and ground-based (Phenotrac IV) systems were studied and the performance of spectral indices was studied, taking into account the importance of N content and biomass for detecting the N uptake in wheat.

Section *III* defines agronomically-based error limits for the spectral detection of N-related traits (aboveground and grain N uptake, and NNI) as well as grain yield in maize. Therefore, a two-year nitrogen increase experiment was conducted at one site. In addition, the suitability of UAV-derived spectral indices to capture the N-related traits and grain yield was evaluated.

3 Materials and Methods

The following paragraphs provide important information on the methods used in Sections *I–III*. For details, the reader is referred to the individual articles indicated in paragraph 4.

3.1 Field trials

Field trials were conducted for Section *I* in 2018 and 2019, for Section *II* in 2020, and for Section *III* in 2018 and 2019.

Figure 5: N-fertilization experiments (Section *I*) in winter wheat in 2018 at the Dürnast research station of the Technical University of Munich (Background: Weihenstephan campus).

In Section *I*, soil sampling for N_{min} analysis was performed on twelve fields, located in different typical agricultural arable farming regions in Southern Germany (*Table 1*). Additionally, nitrogen fertilization experiments were carried out at two different sites (F1, H). Site F1 was located at the Dürnast research station of the Technical University of Munich in Germany (48°23′60″ N, 11°41′60″ E) (*Figure 5*). The average precipitation is approximately 800 mm, the yearly temperature 8 °C, and the soil consists of a mostly homogeneous Cambisol with a silty-clay loam texture. At site H, the average precipitation is approximately 1000 mm, the yearly temperature 8.4 °C, and the soil consists of a Colluvisol with a silty loam texture. All fields were managed conventionally in compliance with local standards and a sufficient supply of all nutrients, except nitrogen, was ensured. One field experiment in Section *II* and all field experiments in Section *III* were conducted at the same site as F1. A further technical description of the nitrogen fertilization experiments is given in *Table 2*.

Table 1: Characterization of the sampling sites. Letters display locations, numbers show different fields at the same location, (1) sL = sandy loam, lS = loamy sand, L = loam, Mo = peat, Lö = loess, Al = alluvium, D = diluvium, (BAYERISCHES LANDESAMT FÜR UMWELT (LFU), 2019) (2) WRB = IUSS WORKING GROUP W.R.B. (2007).

Field	Year of sampling	Coordinates (GPS)	Field size (ha)	German soil assessment data(1) and soil taxonomy according to WRB(2)	Topography
A	2018	48°47'40.0"N 12°47'10.6"E	2.5	L, Lö; Cambisol, stagnic	Plane
B1	2018	48°46'24.6"N 12°41'04.8"E	12.7	L, Lö; Cambisol stagnic	Hilly
B2	2018	48°46'22.4"N 12°40'11.9"E	4.0	L, Lö; Cambisol stagnic	Plane
C1	2018	48°44'46.1"N 11°08'36.2"E	2.7	L, Lö; Cambisol stagnic	Hilly
C2	2018	48°45'07.8"N 11°09'09.2"E	2.4	sL, Lö to L, Lö; Cambisol stagnic	Hilly
D1	2018	48°11'15.8"N 10°59'35.6"E	2.8	L, Lö, D; Cambisol stagnic	Plane
D2	2018	48°11'01.2"N 11°00'13.2"E	2.5	L, Lö, D; Cambisol stagnic	Plane
E	2018	48°10'51.7"N 11°44'07.3"E	3.7	sL, D; Leptosol, skeletic, humic	Plane
F1	2018	48°24'11.9"N 11°42'11.7"E	12.2	L, D; Cambisol stagnic	Hilly
F2	2018	48°24'06.9"N 11°42'26.5"E	4.7	L, D; Cambisol stagnic	Hilly
G	2018	48°14'22.4"N 11°27'46.1"E	5.4	Mo, lS, Al; Fluvisol, gleyic, calcaric, humic	Plane
H	2019	48°10'19.8"N 10°59'25.7"E	1.0	L, D; Cambisol stagnic	Plane

Table 2: Technical description of the N-fertilizer experiments. N-fert. I, II, and III refer to the individual nitrogen split applications. VB indicates the beginning of vegetation.

		2018		2019		2020
Section		*I*	*III*	*I*	*III*	*II*
Investigated crop		Winter wheat (*Triticum aestivum* L.)	Maize (*Zea mays* L.)	Winter wheat (*Triticum aestivum* L.)	Maize (*Zea mays* L.)	Wheat (*Triticum aestivum* L.)
Variety		Reform	Amagrano	Spontan	Amagrano	Apostel
Pre-crop		Rapeseed	Winter wheat	Maize	Winter wheat	Spring barley
Sowing density (kernels m^{-2})		330	11	340	9	350
Experimental design		completely randomized	completely randomized	completely randomized	double-created Latin square	randomized complete block design
Replicates (n)		4	6	4	for each 4	4
Plot length and width (m)		20 x 12	20 x 12	10 x 2	15 x 12	10.5 x 1.5
N-fertilization: growth stages	N-fert. I	VB	Leaf development	VB	Leaf development	VB
	N-fert. II	Begin stem elongation		Stem elongation		Stem elongation
	N-fert. III	Flowering		Heading		Booting
N-fertilization: amount (kg N ha^{-1})	N-fert. I	0/40/60/40/90/60	0/80/120/160	0/45/60/75	0/80/120/160	0/35/40/45/50/55/60/65/70/75
	N-fert. II	0/60/60/90/40/90		0/45/60/75		0/35/40/45/50/55/60/65/70/75
	N-fert. III	0/50/60/80/80/80		0/45/60/75		0/35/40/45/50/55/60/65/70/75
N-fertilization: N-form		Ammonium nitrate	Ammonium sulfate urea	Ammonium nitrate	Ammonium sulfate nitrate	Calcium ammonium nitrate
Fertilizer spreader		Pneumatic spreader, Rauch® AERO, Germany (*Figure 6*)	Pneumatic spreader, Rauch® AERO, Germany	Disc spreader, Bogballe® M35W, Denmark	Box spreader, Fiona® G-85, Denmark	Box spreader, Fiona® G-85, Denmark

Figure 6: N-fertilizer application with the Rauch® AERO pneumatic spreader in winter wheat.

3.2 Weather conditions

The weather data given in *Figure 7* refer to the field experiments in maize in 2018 and 2019 (Section *III*) and the wheat experiment in 2020 of Section *II*.

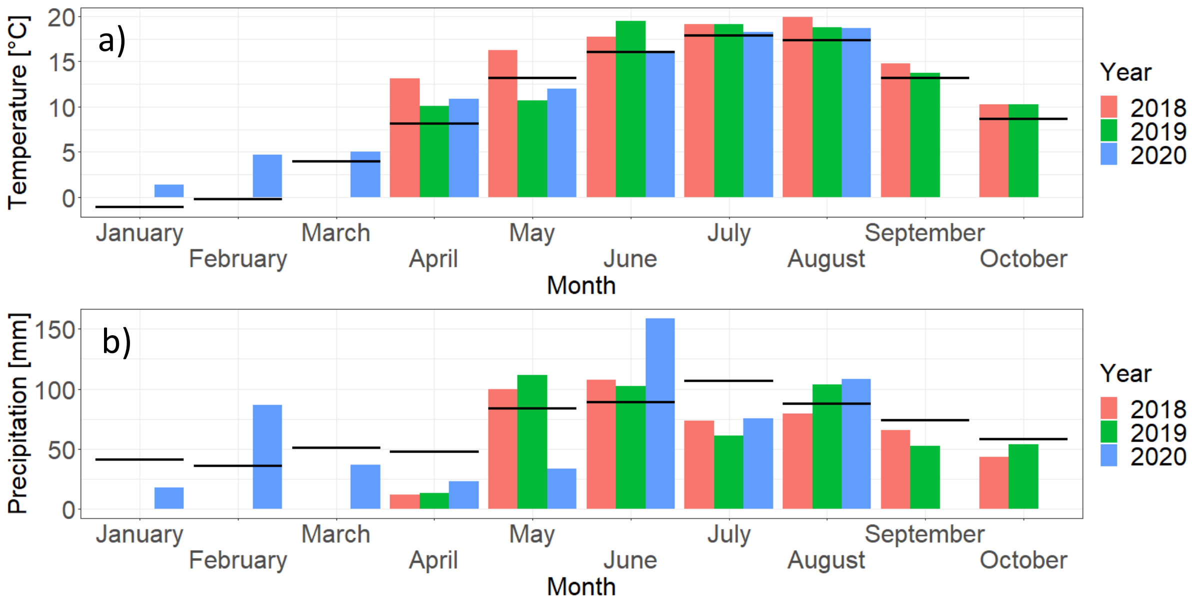

Figure 7: Crop growth relevant monthly weather conditions (January to October) at the experimental site (Dürnast research station, Southern Germany) in 2018, and 2019 in maize and 2020 in wheat. The temperature (a) and precipitation (b) are shown as bars and the long-term average (mean 1981–2010) as lines (CDC, 2020).

The weather conditions in 2018 and 2019 deviated significantly in some of the maize growth relevant months from the long-term average (mean 1981–2010). Both years showed temperatures above the

long-term average in all months, except for May 2019. Comparing both years, 2018 deviated stronger from the long-term average than 2019. Less precipitation was observed in 2018 and 2019 in April, July, August, and September, and in 2018 also in October, and more precipitation was observed in 2018 and 2019 in May and June, and in 2019 also in August compared to the long-term average. Averaged across all months, the total precipitation in 2018 and 2019 was 480 and 498 mm, which was very similar, but indicated a precipitation deficit for both years compared to the long-term average (550 mm).
Also in 2020, significant deviations from the long-term average (mean 1981–2010), which impacted the growth of wheat, could be observed. Temperatures above the long-term average were observed between January and April inclusive and also in August, with the largest differences in February and April. Less precipitation was observed in January, March to May inclusive, and July, and more precipitation in February, June, and August. The strongest deviations are related to February, May, and June.

3.3 Soil and plant sampling, sample analysis, and calculation of soil and plant traits

In Section *I*, a sampling grid for soil sampling was designed for each field to consider the field size and shape using ArcGIS (ESRI®, Germany, Version 10.5.0.6491). Peripheral areas and headlands were not considered. A minimum distance of at least 20 m between sampling points was chosen to avoid the spatial dependence of nitrate-N or N_{min} values (DAHIYA ET AL., 1985; VAN MEIRVENNE AND HOFMAN, 1989; SCHMIDHALTER ET AL., 1991a; ILSEMANN ET AL., 2001). For larger fields, the distance was extended and reduced on smaller fields to achieve an exact representation of the fields and avoid unnecessary soil samplings. Sampling was performed shortly before the beginning of the vegetation for wheat in February and for maize in April. The total soil sampling depths ranged from 60 to 90 cm in agreement with a recently suggested recommendation by the federal advisory institutions (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2018b). One field (E, *Table 1*) could only be sampled down to 30 cm due to the high skeleton content. At all fields except site F, soil samples were taken with a set of two gauge augers (Pürckhauer, inner diameters of 2.5 cm for 0–30 cm and 2.0 cm for 30–60 cm depth), and, corresponding to site F, a tractor-mounted soil sampling device (inner diameter of 3.5 cm for all soil depths) was used. Each sampling point consisted of 2–5 soil samples because the generated soil quantity per sample depends on the soil. The collected soil samples were stored cooled in ice boxes during transport and afterward, if necessary, homogenized and finally frozen for storage until analysis.
To determine the nitrate-N content of each soil sample, 80 g of soil were weighed in performed as duplicate in polyethylene bottles, and 160 mL of calcium chloride solution ($CaCl_2$; 0.01 M) was added to each soil sample and shaken overhead for 60 minutes. Subsequently, the solution was filtered (150 mm, 80 g/m², AHLSTROM MUNKSJÖ®, Helsinki, Finland), and the first part of the filtrate was discarded.

According to VILSMEIER (1984), chemical analysis was carried out using high-performance liquid chromatography (HPLC) and for further calculation of the soil nitrate-N content, a dry bulk density of 1.5 g cm^3 was assumed.

Plant samples of wheat (Sections *I* and *II*) and maize (Section *III*) were manually sampled in an indicative area from each plot at indicative growth stages (BBCH codes, “**B**iologische **B**undesanstalt, Bundessortenamt und **CH**emische Industrie”; MEIER, 2018) to assess the nitrogen status. Plant samples of maize were post-harvest separated into leaves, stems, and if necessary, cobs and afterward chopped. The dry weight, expressed as t ha^{-1}, was determined based on oven-dried subsamples. Afterward, the dried samples were then milled to a fine powder (Brabender®, Duisburg, Germany; Retsch®, Haan, Germany) and subsequently analyzed by a mass spectrometer with an ANCA SL 20–20 preparation unit (Europe Scientific®, Crewe, UK) to ascertain the N content (% of dry weight). The N uptake (kg N ha^{-1}) was calculated as dry weight x N content. In Sections *I* and *III* interior plant rows were threshed (Deutz-Fahr®, Germany) to determine the grain yield (14 % moisture). The grain sample preparation was carried out comparable to the biomass samples and for wheat, the crude protein content was calculated as N content grain * 5.7 (ISO 16634–2, 2016).

For a better understanding of the nitrogen supply of the crops, the nitrogen nutrition index (NNI) (LEMAIRE AND GASTAL, 1997) was calculated in Section *II* for wheat (JUSTES ET AL. 1997) and Section *III* for maize (PLÉNET AND LEMAIRE, 1999) as follows:

Eq. 1: $\mathrm{NNI} = \frac{\mathrm{Nact}}{\mathrm{Nc}}$

where N_c (%) is the critical nitrogen content and N_{act} (%) is the actual measured nitrogen content of the shoot dry matter.

3.4 Spectral measurements

To investigate the relationship between residual soil mineral N values and in-season multispectral satellite images, bottom of atmosphere images from Sentinel-2 were used (Section *I*). These orthorectified and atmospherically corrected surface reflectance data were downloaded from the Google Earth Engine. A detailed technical description of the Sentinel-2 satellite is given by SEGARRA ET AL. (2020). The boundaries of the investigated fields (*Table 1*) were selected as the image section and pixels at the edge of the fields that were not 100 % within the field boundaries were removed. Subsequently, these pixels were interpolated using the nearest neighbor pixels (equal weighting) by regression based on k-nearest neighbors. Only cloudless images were used. In these images, the previously georeferenced nitrate-N sampling points were located, and a buffer, formed as a circle (radius 10 m), was created around each sampling point. The circle reflectance value for each band collected in this way arises from the weighted average (area fraction) of all neighboring pixels. The observation period was April to June for wheat and April to July for maize. Due to the close distance of sampling points in some fields, only high-resolution bands (4–7 and 9) of the Sentinel-2 were used.

In Section *III*, only aerial-based measurements (UAV) were conducted under cloudless conditions to capture N-related traits and grain yield of maize. All observations were done directly after destructive data collection except for the measurement date at BBCH 86 in 2019, where plant sampling was made seven days after the spectral sensing. The flights were performed with the fixed-wing aircrafts eBee and eBee RTK (SenseFly®, Lausanne, Switzerland). Both UAVs were equipped with the same multispectral camera (Sequoia^{+} camera, Parrot, Paris, France). Four spectral bands of the electromagnetic spectrum were recorded: GREEN (550 nm, ~40 nm bandwidth), RED (660 nm, ~40 nm bandwidth), REDEDGE (735 nm, ~10 nm bandwidth), and NIR (790 nm, ~40 nm bandwidth). For calibration, a white balance card was used. The flights were carried out in 2018 and 2019 at heights of 80 and 55–60 m above the ground, resulting in ground resolutions of about 8 and 5 cm/pixel. Pix4D software (Pix4D S.A., Prilly, Switzerland) was used to merge the individual images. Further details of the UAV equipment are given in HU ET AL. (2020b). Based on the complete image, a polygon for each plot and the individual band was created using ArcGIS (ESRI®, Germany, Version 10.5.0.6491). Care was taken to exclude peripheral and biomass harvesting areas and polygons affected by artifacts.

The aerial-based measurements and the further processing of the spectral data in Section *III* were the same as in Section *II*, except for the use of the fixed-wing aircrafts eBee X (BBCH 37) and eBee Plus (BBCH 61) (SenseFly®, Lausanne, Switzerland). For ground-based measurements, the vehicle sensor platform Phenotrac IV (BARMEIER AND SCHMIDHALTER, 2017b) equipped with a hyperspectral bidirectional passive sensor spectrometer (tec5®, Oberursel, Germany) mounted at the front center was used. The measuring range of the sensor is 300 to 1000 nm with a nominal resolution of approximately 3.3 nm, and a field of view (FOV) of 24°. Field measurements were conducted with a distance to the canopy surface of approximately 0.8 m and a driving speed of approximately 5 km h^{-1}. Other ground-based measurements were performed with the handheld sensors Handy-Spec® field spectrometer (LI ET AL., 2012) and a two-channel spectrometer (WESTERMEIER AND MAIDL, 2019). A more detailed description of these handheld sensors can be found in the publications indicated. All reflectance data were used to calculate commonly used indices (*Table 3*), including wavelengths related to maize traits (MISTELE AND SCHMIDHALTER, 2008a; ZHAO ET AL., 2018; RAMOS ET AL., 2020; GARCÍA-MARTÍNEZ ET AL., 2020), and wheat traits (MISTELE AND SCHMIDHALTER, 2008b; MISTELE AND SCHMIDHALTER 2010; ERDLE ET AL., 2011; PREY AND SCHMIDHALTER 2019c; DE SOUZA ET AL. 2021).

Table 3: List of spectral indices. Depending on the technique used, the original published spectral wavelengths were approximated.

Section	Index	Equation	Sensor platform	Reference
I, II, III	NDVI	$\frac{R790 - R660}{R790 + R660}$	UAV, Phenotrac IV, Sentinel-2	ROUSE ET AL. (1974)
II, III	NIR/GREEN	R780/R550	UAV	MISTELE AND SCHMIDHALTER (2008a, 2008b)
II, III	NIR/RED	R780/R670	UAV	GITELSON ET AL. (2003)
II, III	NIR/REDEDGE	R780/R735	UAV	DE SOUZA ET AL. (2021)
II, III	NDRE	$\frac{R790 - R720}{R790 + R720}$	UAV	BARNES ET AL. (2000)
I, II	REIP	$700{+}40\left(\frac{\left(\frac{R670+R780}{2}\right)-R700}{R740-R700}\right)$	Phenotrac IV, Sentinel-2	GUYOT ET AL. (1988)
II	R760/R730	R760/R730	Phenotrac IV	ERDLE ET AL. (2011)
II	R780/R740	R780/R740	Phenotrac IV	MISTELE AND SCHMIDHALTER (2010)

3.5 Data analysis and further calculations

Data analysis across all sections was performed with Microsoft® Excel® 2019 MSO (16.0.12527.20260), IBM® SPSS® Statistics 26 software, and R (2018, 2021).

In Section *I*, the following statistics were calculated for soil data: mean value, standard deviation, minimum and maximum value, coefficient of variation (CV [%] = standard deviation/mean value*100), linear regressions, and Pearson correlations (KÖHLER ET AL., 2012). The Shapiro-Wilk test was used to check the normal distribution of the data. Equation 1 calculates the number of soil samples (n) that must be taken to be within d units of the mean value:

Eq. 1: $n = X_{\alpha}^{2} * \sigma^2 / d^2$

where X_{α} is the standard normal distribution, σ is the standard deviation and d indicates the acceptable error (absolute value in kg nitrate-N ha^{-1}) of the mean value. A further analysis concerned the comparison of the regionally aggregated N_{min} values from the official advisory system (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2018a and BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2019) with a reduced sampling intensity (restricted to two samplings per area for a soil depth of 0–60 cm). For the field nitrogen fertilization experiments, nitrogen use efficiency, nitrogen uptake efficiency, nitrogen utilization efficiency (LÓPEZ-BELLIDO ET AL., 2005), N-balance (simplified according to OECD AND EUROSTAT, 2007), and nitrogen harvest index (DELOGU ET AL., 1998) were calculated as efficiency parameters. A further economic evaluation includes the N-free output (KARATAY ET AL., 2018) using wheat prices according to BUNDESMINISTERIUM FÜR ERNÄHRUNG UND LANDWIRTSCHAFT (2019) and an assumed price for fertilizer nitrogen of 1 € per kg nitrogen. For details, the reader is referred to the original publication (Section *I*).

In Sections *II* and *III*, based on the Akaike Information Criterion (AIC) (WEBSTER AND MCBRATNEY, 1989), either linear or polynomial (second-order) regressions were calculated and the coefficient of determination (R^2) was used as a measure of the goodness of fit. R^2 indicates the portion of the explained variance in the model regarding the total variance (Eq. 2):

Eq. 2: $R^2 = \frac{explained\ deviation\ sum\ of\ squares}{total\ deviation\ sum\ of\ squares\ to\ be\ explained} = \frac{\sum_{i=1}^{n}(\hat{y}i-\bar{y})^2}{\sum_{i=1}^{n}(yi-\bar{y})^2}$

where $\hat{y}_i$ is the estimator (regression function) of each observed y_i and $\bar{y}$ is the arithmetic mean of all observed y_i. For a better understanding, *Figure 8* illustrates these relationships graphically.

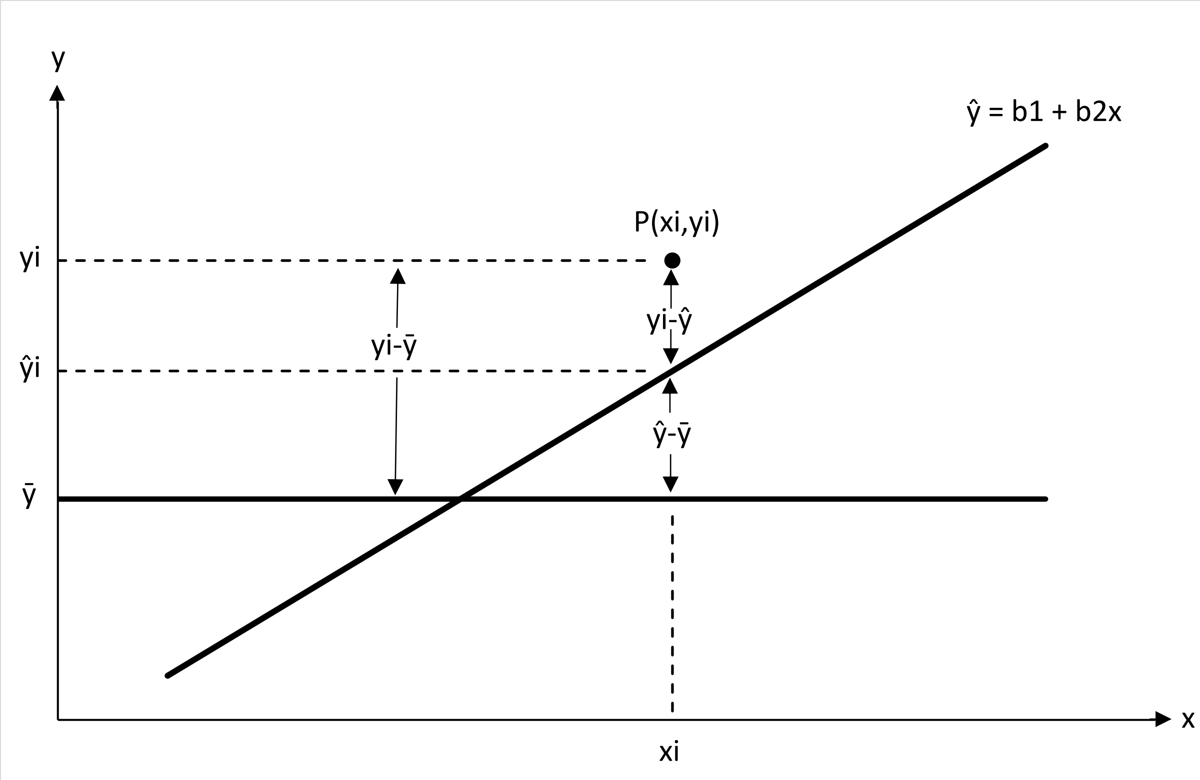

Figure 8: Diagram showing the decomposition of the deviation sum of squares, where x and y represent the independent and dependent variables with P as an example of a single measured value, $\hat{y}_i$ is the estimator (regression function) of each observed y_i and $\bar{y}$ is the arithmetic mean of all observed y_i (BLEYMÜLLER ET AL., 2008).

As a further measure of the predictive quality of the regression, confidence and prediction intervals (95 % level) were calculated (BLEYMÜLLER ET AL., 2008; KÖHLER ET AL., 2012). Additionally, the root mean square error (RMSE) was calculated as follows:

Eq. 3: RMSE [kg N ha^{-1}] = $\sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}}$

where O_i are the measured and P_i the predicted values for the N uptake and n the number of samples. For a better understanding it should be mentioned that P_i is equal to $\hat{y}_i$ and O_i is equal to y_i (*Figure 8*).

To enable better comparability of RMSE with other data sets, the standardized RMSE [%] (modified according to LOAGUE AND GREEN, 1991) was calculated as follows:

Eq. 4: RMSE [%] = $\sqrt{\frac{\sum_{i=1}^{n}(P_i - O_i)^2}{n}}$ x $\frac{100}{\bar{O}}$

where O_i and P_i are observed and predicted values and n the number of samples, whereas $\bar{O}$ represents the mean of the observed data. Afterward, the RMSE values were classified and evaluated according to WESTERMEIER AND MAIDL (2019). RMSE values < 10 % were rated as excellent, 10–20 % good, and > 30 % sufficient.

Another widely used and generally accepted error in the entire model is the mean absolute error (MAE), which was calculated as follows:

Eq. 5: MAE [kg N ha^{-1}] = $\frac{\sum_{i=1}^{n}|P_i - O_i|}{n}$

where O_i and P_i are observed and predicted values, and n is the number of samples (WILLMOTT 1984).

Additionally in Section *II*, Pearson correlations (*r*) as well as the partial correlation coefficient were calculated (BACKHAUS ET AL., 2006; KÖHLER ET AL., 2012). The partial correlation coefficient eliminates the influence from one additional variable (covariate) and is given as:

Eq. 6: $r_{x1,x2|\xi}$ = $\frac{r_{x1,x2} - r_{x1,\xi} \cdot r_{x2,\xi}}{\sqrt{(1 - r_{x1,\xi}{}^{2}) \cdot (1 - r_{x2,\xi}{}^{2})}}$

where $r_{x1,x2}$ are the correlation coefficients between $x1$ and $x2$, $r_{x1,\xi}$ are those between $x1$ and ξ and $r_{x2,\xi}$ are the ones between $x2$ and ξ. If the additional variable does not influence the correlation of the other two variables, the partial correlation coefficient is at the same level as the Pearson correlation coefficient (without the covariate). Increasing influence is indicated through a lower partial correlation coefficient and the difference between the Pearson and the partial correlation coefficient is equal to the influence of the covariate.

Sections *II* and *III* included, in addition to the commonly accepted statistical error measures for regressions, confidence intervals that tolerate a model error that is acceptable from an agronomic point of view. This error was calculated as follows:

Eq. 7: agronomic error [unit of the trait of maize and wheat] = $\hat{y}_i$ ± error of y_i

where y_i is the agronomic error and $\hat{y}_i$ is the estimator of the regression function. As a measure of goodness, the proportion of data points that fell inside the interval was chosen, and, we imply that a reasonable value is at least 80 %.

4 Manuscript overview

4.1 Section *I*: Simplifying residual nitrogen (N_{min}) sampling strategies and crop response

Heinemann P., Schmidhalter U., 2021. Simplifying residual nitrogen (N_{min}) sampling strategies and crop response. European Journal of Agronomy, 130. 126369. doi.org/10.1016/j.eja.2021.126369.
URL: https://www.sciencedirect.com/science/article/pii/S1161030121001404.

Author contributions

Paul Heinemann: Investigation, Methodology, Data curation, Formal analysis, Writing - original draft. Urs Schmidhalter: Conceptualization, Supervision, Writing - review & editing, Project administration, Funding acquisition.

Summary

World-wide, decisions concerning the N-fertilization of crops occur at early growth stages when plant development is less and not indicative of their demands. Therefore, optimizing nitrogen fertilization requires the evaluation of the available soil mineral nitrogen content (N_{min}) early in the season. In Germany, areas characterized by increased nitrate concentrations in the groundwater (approximately 28% of the arable land) require since 2020 a mandatory soil N_{min} analysis for each crop on a representative field. In this context, optimization of soil analysis is needed because it is costly, time-consuming, and labor-intensive.

This work investigated maize fields in 2018 and wheat fields in 2018 and 2019, where soil sampling was carried out in a grid pattern in spring. The soil nitrate-N content was determined for each 30 cm layer, and in total down to a soil depth of 60 cm in 11 fields and further down to 90 cm soil depth in two of the fields. Given a deviation of less than 10 kg nitrate-N ha^{-1}, each single and the combined soil depths of all fields could be sampled only with two soil samples. Generally, the reduced field-specific soil sampling strategy even performs more precise N_{min} values by 11.2 kg nitrate-N ha^{-1} for wheat fields and, slightly less precise values by 4.8 kg nitrate-N ha^{-1} for maize fields, however. This proved to be beneficial compared to crop-specific, regionally representative N_{min} values offered by the official advisory authorities. Further investigations of nitrogen fertilization experiments supported the applicability of the new simplified N_{min} strategy. The findings are valid for conventional tillage managements and relative homogeneous fields with field sizes in the range of 1.0–12.7 ha. A replacement of soil analysis through multispectral in-season satellite imagery from Sentinel-2 was not feasible. In combination with available simplified on-farm analysis of the soil nitrate content, a more intensive field-specific soil N_{min} analysis contributes to improved nitrogen management, decreases adverse environmental effects, and saves analysis and sampling costs.

4.2 Section *II*: Evaluating and defining agronomically relevant detection limits for spectral reflectance-based assessment of N uptake in wheat

Heinemann P., Haug S., Schmidhalter U., 2022. Evaluating and defining agronomically relevant detection limits for spectral reflectance-based assessment of N uptake in wheat. European Journal of Agronomy, 140. 126609. doi.org/10.1016/j.eja.2022.126609.

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Author contributions

Paul Heinemann: Conceive & design & implementation of the experiment, Data analysis, Writing – original draft & review & editing

Stephan Haug: Statistical supervision, Writing - review & editing

Urs Schmidhalter: Conceive & design of the experiment, Writing - review & editing, Project administration, Funding acquisition.

Summary

The spectral determination of the N uptake of wheat is a commonly used method as it is cost-efficient, rapid, and non-destructive. Nevertheless, there exists a lack of agronomical-based spectral detection limits. Currently used statistical measures such as R^2, RMSE, or MAE do not fully satisfactorily address the agronomical relevance, especially when sensing is frequently carried out under extreme N supply conditions which may not reflect current farming practice. The present study, therefore, used different data sets covering several years, sites, varieties, and developmental stages of wheat (*Triticum aestivum* L.), to evaluate regression models between the N uptake and commonly used spectral indices, sensed from hyperspectral ground-based and multispectral unmanned aerial vehicles (UAV). The results suggest that an evaluation through commonly used statistical measures is not sufficient from an agronomic point of view. The R^2 is essentially influenced by differentiating N uptake which is frequently linked to later growth stages. Further statistics such as RMSE and MAE only average the error, which leads to an under- as well as overestimation for most observations, and should therefore be extended by agronomic-based error intervals. In this investigation, we defined, based on a probability of at least 80 %, a suitable error interval of ± 15 kg N uptake ha^{-1} up to BBCH 50. The interval limits can be closer in earlier developmental stages and wider at later growth stages. In addition, this research pointed out that extreme N levels can bias the models and should be limited to N-fertilization ranges that are indicative of the current site-specific farming practice. For detecting N uptake, differentiation of biomass is more important than that of N content. Terrestrial- as well as UAV-based sensing were equally suitable for detecting the N uptake of wheat when spectral bands of the REDEDGE and NIR regions were combined. In general, agronomically-based detection limits facilitate the evaluation and should be included besides common statistical measures in the spectral valuation of wheat N uptake.

4.3 Section *III*: Spectral assessments of N-related maize traits: Evaluating and defining agronomic relevant detection limits

Heinemann P., Schmidhalter U., 2022. Spectral assessments of N-related maize traits: Evaluating and defining agronomic relevant detection limits. Field Crops Research, 289. 108710. doi.org/10.1016/j.fcr.2022.108710.

URL: https://www.sciencedirect.com/science/article/pii/S0378429022002817?dgcid=author.

Author contributions

Paul Heinemann: Investigation, Methodology, Data curation, Formal analysis, Writing - original draft. Urs Schmidhalter: Conceptualization, Supervision, Writing - review & editing, Project administration, Funding acquisition.

Summary

Spectral sensing is a widely used method in agriculture to detect N-related traits and the grain yield of maize (*Zea mays* L.) because it is non-destructive, rapid, and cost-efficient. However, to date, a lack of knowledge of agronomically supported spectral detection limits exists. Commonly used statistical measures such as R^2, RMSE, and MAE do not fully satisfactorily consider the agronomic relevance and should therefore be extended. The present study evaluated regression models of spectral indices derived from an unmanned aerial vehicle (UAV) by capturing grain and aboveground N uptake, NNI, and grain yield covering data sets of two sites, years, and four developmental stages of maize. The results suggest that an agronomic evaluation exclusively based on widely used statistical measures is not fully adequate. The R^2 is essentially affected by the differentiation of the trait, which in turn depends on growth stages and year effects. Further commonly used statistics such as MAE and RMSE only average the error and therefore lead to an over- as well as underestimation for most observations. In this study, we defined a suitable agronomical error interval for grain and aboveground N uptake, nitrogen nutrition index, and grain yield of ±25 and ±40 kg N ha^{-1}, ±0.2, and ±1.4 t ha^{-1}, in compliance with a probability of at least 80 %. These error intervals are consistent across growth stages and years because most spectral indices are mainly dominated by the biomass of maize. Across all of them, spectral indices perform best when combinations of GREEN, REDEDGE, and NIR bands are used. For spectral indices using the RED band, the range of the agronomic error interval performed equally, but with a slightly higher probability of data points outside the error limits. Common statistical measures should be extended by agronomically-based error limits in the spectral assessment of N-related traits of maize and grain yield to optimize the ex-ante and/or ex-post analysis of N-fertilization.

5 General discussion

Chapters 5.1–5.3 discuss the results reported in Section *I*. Chapters 5.4–5.6 and 5.8 address the findings of Sections *II* and *III*. Chapter 5.7 discusses further results only observed in Section *II* whereas chapter 5.9 encompasses future aspects.

5.1 Simplified residual soil nitrogen sampling strategy

An exact determination of the soil mineral N content depends on diverse factors such as, e.g., an incorrect estimation of the stone content (SCHARPF, 1977), assumption of an incorrect bulk density, insufficient representativeness of soil sampling and sample treatment (MOLITOR, 1982), and also the influence of the sampling device (BAKER ET AL., 1989). When calculating the N_{min} value, the possible error of an incorrect estimation of the bulk density and the soil's stone content may be higher than the analytical error (SCHMIDHALTER ET AL., 1991a, 1991b), which was quantified in total (storage, transport, and soil sample preparation) by RICHTER ET AL. (1984) in the range of 10–15 kg NO_3^- N ha^{-1}. Additionally, they evaluated an analytical error of UV spectrometry up to 5.5 kg nitrate-N ha^{-1}. BAKER ET AL. (1989) pointed out that smaller diameters of the sampling devices led to lower NO_3^- N ha^{-1} values and the earth auger with 5.1 cm was most suitable. Because several soil samples have been collected to produce the required amount of soil at one sampling point in this study, the error of small-scale variability is important too. This error was determined by GIEBEL ET AL. (2006) with 10.2 to 26.5 kg ha^{-1} for N_{min}-N and a soil depth of 0–60 cm at sampling distances smaller than 6 m and could be caused by inhomogeneous distribution of aboveground plant residues and straw, differing mineralization rates, and spatially differing nitrogen uptake as well as incorporation of plant residues. However, the most important error source is non-representative field sampling. In this study, this error was chosen with 10 kg nitrate-N ha^{-1} and seems to be quite practical compared to the error sources just mentioned.

The number of samples per field depends on the confidence interval level (KANWAR ET AL., 1998). Therefore, this study achieved a low risk of incorrect values with the use of a 93 % confidence interval. The result to obtain a representative mean value of mineral nitrogen with only two soil samples per field found in this work largely agrees with other studies. SCHMIDHALTER ET AL. (1991a, 1991b) could determine the field-specific N_{min} mean value for the total depth of 100 cm with five soil samples and an accuracy of ±23 kg ha^{-1}. At two locations, SCHMIDHALTER ET AL. (1992) reported a number of soil samples of 5–13 and 2–6 to achieve sufficient accuracy of the mean value of ±10 and ±15 kg N, respectively. ILSEMANN ET AL. (2001) found required sampling intensities of 9, 16, and 76 soil samples for three different sites with a given deviation of the mean value of less than 10 kg NO_3-N (probability level of 95 %). The increase in the latter value was due to an uneven distribution of liquid manure and therefore indicates a limitation for reduced soil sampling although a homogeneous distribution of organic fertilizers should generally be aimed at and especially before N_{min} soil sampling.

Geostatistical analysis of nitrate-N data provides little additional information than classical statistical methods (STENGER ET AL., 2002). The coefficient of variation (CV) is commonly used to juxtapose the scatter of different samples with dissimilar mean values. However, the study pointed out that a trend between the CVs and mean nitrate-N values exist. This finding is in line with SCHMIDHALTER ET AL. (1991a, 1991b), SCHMIDHALTER ET AL. (1992), and HABERLE ET AL. (2004). Additionally, the study pointed out that the use of the N_{min} mean level is more decisive for the sampling intensity than the CV. SCHMIDHALTER ET AL. (1991a, 1991b) previously reported that even increased variations at somewhat strongly increased nitrate contents are of little relevance because at these high levels, no additional nitrogen fertilization is advised. The relevance is also less if low N_{min} values occur.

For the correct calculation of the number of soil samples per field, the distribution of the data is important because it can influence the correct estimation of the sampling intensity (PARKIN AND ROBINSON, 1992). In this work, frequency distributions of nitrate-N values varied across the soil depths as well as from field to field. SCHMIDHALTER ET AL. (1991a) observed for N_{min} values a log-normal distribution for the subsoil and a normal distribution for the topsoil. VAN MEIRVENNE AND HOFMAN (1989) observed for nitrate-N values log-normal distributions in October and February and normal distributions for April for the soil layer 0–100 cm. STENGER ET AL. (1998) observed constant as well as changing N_{min} distributions in 0–90 cm across individual fields and several years. Thus, it is difficult to identify the distribution of the mineral nitrogen content of the soil in a field because it can be subject to both temporal and spatial variation. Non-normally distributed values might be due to large differences in soil texture, unevenly distributed crop residues, and fertilizers. In addition, the distribution is influenced by the number of soil samples per field. However, each field could be reliably recorded with only two soil samples despite the incorrect assumption of a normal distribution.

In this study, soil sampling occurred on relatively equal-sized fields. The study of VAN MEIRVENNE ET AL. (1990) illustrated the inherent variability of inorganic nitrogen, with results indicating that nitrogen varies considerably and more or less comparably from small (1 m²; RAUN ET AL., 2002) to larger scales (1 ha to tens of hectares; REUSS ET AL., 1977; SCHMIDHALTER ET AL., 1992; GIEBEL ET AL., 2006), with few differences observed irrespective of the availability and the form of nitrogen. Coefficients of variation between 30 and 60 % irrespective of the scale have been described by REUSS ET AL. (1977), and SCHMIDHALTER ET AL. (1992). HABERLE ET AL. (2004) reported that in a 19 ha experimental field, the coefficient of variation of nitrate in the topsoil and subsoil (0–30 and 30–60 cm) ranged from 18 to 39 and 20 to 37 %. Therefore, it seems possible to extrapolate the findings from this study to larger-sized fields, but this needs to be further investigated. The field sizes under investigation varied from 1.0 to

12.7 ha and reflect well the typical situation in the German federal state of Bavaria. Only 5 % of the fields in this region are greater than 5 ha (BAYERISCHE LANDESANSTALT FÜR LANDWIRTSCHAFT (LFL), 2018c). However, the field sizes in other federal states in Germany, e.g. East Germany, are significantly larger (LANDESAMT FÜR LÄNDLICHE ENTWICKLUNG, LANDWIRTSCHAFT UND FLURNEUORDNUNG (LELF), 2021). Thus, the extrapolation of the findings of this study is not recommended without further investigations. Even smaller fields can spatially differ significantly in soil and plant properties (MITTERMAYER ET AL., 2021; SCHUSTER ET AL., 2022; STETTMER ET AL., 2022). Therefore, soil sampling and N management within these heterogeneous fields should be site-specific.

KNITTEL AND FISCHBECK (1979) observed an influence of topography on nitrate-N contents and suspected that this result might be due to the thicker loess layer and the direction of water and nutrient flows. Likewise, FRANZEN ET AL. (1998) reported better results for soil sampling for nitrate-N by topography. In contrast and as in this study, GIEBEL ET AL. (2006) found no influence of topography on the spatial distribution of N_{min} values. For relatively small fields as investigated in this study, topography`s influence on nitrate-N sampling seems to be rather negligible. Otherwise, in the case of two soil samples per field, one can be taken at higher and one at lower elevations.

The correlation between the nitrate-N content of individual soil layers varied site-specifically and nitrate-N contents of lower soil depths could not be estimated from upper soil layers. Although changes in the N_{min} content concerning soil-borne-N during vegetation predominate at 0–30 cm (PESCHKE AND MOLLENHAUER, 1998), WEHRMANN AND SCHARPF (1979) observed at different locations at the beginning of the vegetation only small differences in the topsoil between the sites compared to the subsoil (40–100 cm soil depth) with more marked differences. These different results of the vertical distribution of mineral nitrogen in the soil at the beginning of vegetation, which can markedly vary temporarily and spatially, indicate the necessity to sample the entire soil depth yearly.

The study could clearly show that the soil's field-specific mineral N content could be recorded significantly better by reduced soil sampling (especially for wheat) compared to the N_{min} value of the official advice. The latter is an average value based on large sample size and tended to be much higher and therefore leads to an overestimation of the nitrate-N values. Published regionalized values should be seen only as a rough guide. Due to the limited data basis of maize fields, the comparison should be extended to additional cases. Furthermore, the reduced field-specific soil sampling approach reduces the soil sampling by number and the analysis by combining the soil depths and has great potential for cost reduction.

5.2 Simplified residual soil nitrogen sampling strategy: Applicability in N-fertilization decisions

Two nitrogen fertilizer experiments, conducted on two sides, were used to evaluate the applicability of the simplified residual soil nitrogen strategy. For both sides (fields F1 and H, *Table 1* and *2*), the published official advisory regional-based N_{min} values were well above the soil nitrate-N content values determined by reduced soil sampling. Therefore, a significantly higher N-fertilization would have been possible especially at the first nitrogen top-dressing. The first nitrogen application is influenced by weather and soil, plant development, and the N_{min} value. For example, in the case of a target value of 120 kg N_{min} ha^{-1} is assumed for wheat at the beginning of vegetation (WEHRMANN AND SCHARPF, 1979), the first nitrogen application should be higher if the N_{min} content is low. At site F1, it could be shown that an increased and earlier applied fertilizer nitrogen was mostly absorbed, with levels approximately the same for N uptake efficiency and the important parameters from an environmental point of view (straw N uptake and postharvest nitrate-N content of the soil), increased decisive parameters for the farmer (grain yield, grain protein content, grain N uptake, and monetary income), and levels only slightly worse for all other efficiency parameters and the N balance compared to the nitrogen fertilizer strategy based on official advisory regionally crop-specific aggregated N_{min} values. The field experiment at site F1 was only conducted in 2018 and thus, should not be generalized.

At site H, only the absolute amount of N-fertilization could be considered. Due to favorable weather conditions in 2019 and long-term organic fertilization, both the N-mineralization determined from the official advisory values and the grain yield were underestimated when determining the fertilizer requirement.

Although the use of the N_{min} value at the beginning of vegetation in N-fertilizer requirement determination is only one component, it represents nonetheless an important piece of information for N-fertilizer decisions. For example, PUNTEL ET AL. (2019) highlighted the importance of nitrate in the soil (0–60 cm) as a dynamic variable for modeling the economic optimum N rate and the grain yield in the unfertilized plot for maize. Accurate assumptions in the requirement determination optimize N-fertilization. However, other incorrect assumptions, such as yield expectations or N-mineralization during vegetation, cannot be compensated by more precise field-specific N_{min} sampling.

This study investigated only fields where soil tillage occurred conventionally with basic tillage implements as plow and cultivator. However, especially in the case of no-till practices, many biological, chemical and physical soil parameters differ across soil depths compared to conventional tillage systems (AZIZ ET AL., 2013). Tillage influences the amount as well as the distribution of the different soil N pools (MC CARTY, 1995), and the availability of O_2 to microorganisms is increased in the zone of disturbance (DINNES ET AL., 2002). As a result, nitrate-N values can decrease in the upper soil layers at no-till practices (AL-KAISI AND LICHT, 2004). Therefore, the different vertical distribution of nitrate-N values should be implemented in N management decisions. The suggestion of this study to merge the nitrate-N values of the single soil depths to one single nitrate-N value is more recommended for the determination of the absolute N-fertilization requirement.

5.3 Opportunities to substitute simplified residual soil nitrogen sampling through spectral sensing

Spectral measurements are widely used to detect differences in N-related traits of crops during the vegetation (MISTELE AND SCHMIDHALTER, 2008a; MISTELE AND SCHMIDHALTER, 2008b; SCHMIDHALTER ET AL., 2008; MAYFIELD AND TRENGOVE, 2009; ERDLE ET AL., 2011; RAMOS ET AL., 2020). Likewise, ELSAYED ET AL. (2018) and PREY ET AL. (2018) showed that differences in nitrogen status and biomass can also be spectrally inferred at relatively early growth stages. If small differences in soil N_{min} are reflected in the biomass or nitrogen status of plants, spectral sensing could be used as an alternative to soil sampling.

The results observed in Section *I* showed in general only weak correlations between the spectral indices and the field-wise N_{min} values. Neither the use of the NDVI nor the REIP improved the correlations at the available dates or soil depths across all fields. These results indicate the difficulties of evaluating N_{min} by crop response using spectral information. Crop N uptake is relatively low in the early growth stages when N_{min} assessments are made. Consequently, high soil mineral N contents will not be absorbed by plants and become visible, and low mineral N contents already cover the N-demand of the crops. These circumstances restrict plants as an indicator of the N_{min} status at early developmental stages. Although moderate variation in the soil N_{min} status could be observed in some fields, this will not be reflected in the pursuing biomass growth as evidenced by in-season satellite imagery. Substantial effects on biomass at this time might be due to overlapping seeding areas or differences in field emergence caused by varying soil texture combined also with climatic winter conditions or sowing techniques. During vegetation, plant N uptake might reveal different N_{min} contents but will be masked and influenced by nitrogen fertilization. It is more likely to be detected at very low or omitted nitrogen fertilization and needs further investigation.

5.4 Field experiments: year and site-specific growth of wheat and maize

Due to the relatively dry weather conditions early in the season, a sufficient N-fertilization effect in wheat could not be observed for the N-fertilization Experiment 1 (Section *II*) (*Figure 7*). If top-dressed nitrogen is not moved into deeper soil layers and the topsoil also dries out, the plant will not be able to use any potentially available nitrogen, which possibly results in subsequent N deficiency (HARMSEN, 1984). N deficiency occurs firstly because N concentration in the biomass decreases while the growth rate remains the same, and secondly because the growth rate decreases, thereby reducing the accumulation of dry matter (JUSTES ET AL., 1997). The study observed a reduction of secondary tillers. However, promoted due to sufficient rainfall in June, a subsequent N uptake was favorable for the grain filling phase. Other authors also observed that the effect of N-fertilization on N uptake varies from year to year (DELOGU ET AL., 1998; LÓPEZ-BELLIDO AND LÓPEZ-BELLIDO, 2001). Especially the effects of the first two N-dressings were reported by MAIDL ET AL (1998). N-fertilization at the beginning of vegetation promoted the number of fertile tillers per m², while N-fertilization during stem elongation supported the number of grains per ear. Compared to the average of the previous years, the biomass at this site was significantly lower in 2020. Soil variability can cause an additional variability of biomass because it influences the water holding capacity and plant nutrient supply, as well as other variables affecting plant growth (CRAIN ET AL., 2013). Especially small variations in soil texture and soil cause increasingly large effects on plot-to-plot variability under limiting soil moisture conditions (CECCARELLI AND GRANDO, 1996).

The growth of maize (Section *III*) was favorably supported by the prevailing temperatures. Extremely high temperatures above 30 °C, which might negatively influence maize growth (STEWART ET AL., 1998), were not observed. In addition, the lower precipitation level was considered to have had little effect on maize growth because the soil (Cambisol) at this site has a high available field water capacity (down to 100 cm soil depth of around 241 mm), which is attained at the beginning of vegetation and buffers a possible lack of precipitation (HEIL ET AL., 2020). The high influence of year effects and soil factors on maize growth were also reported in other studies (DI PAOLO AND RINALDI, 2008; BERENGUER ET AL., 2009; CORRENDO ET AL., 2021). The study observed an astonishing high N supply of the soil in both years. However, this is in line with CASSMAN ET AL. (2002), who reported an indigenous N supply of 80–240 kg N ha^{-1} for maize. OSTERHOLZ ET AL. (2017) observed that the daily N uptake of maize was exceeded by the daily gross ammonification rate of the soil. It is further suggested that maize can cover its N uptake through the efficient utilization of this N source in competition with soil microbes. Although no organic fertilization was carried out in the experimental fields, the necessary organic matter would have been present. QUAN ET AL. (2021) emphasized the importance of soil organic C in increasing N use efficiency although not a sufficient N replenishment exists through a high proportion of organic matter in the soil. In Europe, upwards of 40% of the N uptake of maize is derived from N-fertilizers. Also, an effect of N-fertilization existed in this study and was evident from the increased N uptake in the fertilized variants.

5.5 Use of conventional statistical measures of goodness in the evaluation of the spectral detection of N-related traits of wheat and maize

A commonly statistical method to model the spectral detectability of N-related traits of wheat and maize is regression analysis. Subsequently, the performance of the models was evaluated based on the coefficient of determination (R^2) (MISTELE AND SCHMIDHALTER, 2008a; MISTELE AND SCHMIDHALTER 2010; ERDLE ET AL., 2011; WINTERHALTER ET AL., 2011; LI ET AL., 2012; MARESMA ET AL., 2016; CORTI ET AL., 2019). The expression of the R^2 depends mostly on the differentiation of the respective trait. A differentiation occurs through the treatment effect (e.g., N-fertilization), which in turn depends on the location (e.g., soil), year (weather), and mainly on the growth stage of the crop on the date of measurement. The influence on the R^2 is probably given because the proportion of the explained deviation sum of squares increases more than the total deviation sum of squares to be explained. Only slight treatment effects through different nitrogen applications, which increased during the vegetation, and thus resulted in higher R^2 values, were observed for maize (Section *III*) which is in line with CORTI ET AL. (2019). Similar observations could be made in the field experiment in wheat in Section *II*. However, high R^2 values alone do not generally imply a sufficient spectral detection of N-related traits from an agronomical point of view.

In a further step, additional statistical measures such as the root-mean-square error (RMSE), standardized RMSE, and the mean absolute error (MAE) are often also used to evaluate the model's performance. A well-performing regression model to estimate the dependent parameters (e.g., N-related traits) is assumed when high R^2 and low RMSE and MAE values occur (LEE ET AL., 2020; ZHANG ET AL., 2020). RMSE and MAE have the advantage that the given model error has the same unit as the target trait. The RMSE averages the squared deviations, whereas the MAE averages the absolute deviations. RMSE values are larger than the MAE values because squaring the errors weights the measured values further away from the regression equation more heavily. This could also be observed in Sections *II* and *III* and is in line with KAYAD ET AL. (2019). Nevertheless, RMSE and MAE average the model error, which leads to both over- and underestimations of the measured values. In general, high R^2 values are mostly associated with lower RMSE and standardized RMSE values (NGUY-ROBERTSON ET AL., 2012; XIA ET AL., 2016; LEE ET AL., 2020; LI ET AL., 2020; SKAKUN ET AL., 2021).

Therefore, an extension of commonly used measures of goodness should be considered to evaluate regression models from an agronomical perspective.

5.6 Consideration of agronomical aspects in the spectral assessment of N-related traits of maize and wheat

The advantage of agronomical intervals is that they are self-defined because the interval limits may vary depending on the trait, year, site conditions (e.g., N-fertilization levels or yield expectations), and also from the interest of application (ex-ante and/or ex-post analysis). For example, a window for in-season management decisions (ex-ante) is defined by THOMASON ET AL. (2007) in the range between the five to nine and by MORRIS ET AL. (2018) in the range between the six to twelve leaf developmental stage for maize. Additionally, ex-post evaluations (e.g., grain yield and/or aboveground N uptake differentiation through diversification of N-fertilization levels) can also provide useful information. According to these approaches, the range of the agronomic interval can therefore be adjusted and the evaluation of the model performance can occur based on the level of probability that the measured values are within or outside the interval. In all cases, the evaluation of the applicability of the spectral detection of maize traits was supported.

If N-fertilization applications in wheat are based on spectral information, the detection error should be as small as possible. Depending on the growth stage of wheat, two error intervals ($\hat{y}i \pm 10$ and ± 15 kg N uptake ha^{-1}) were chosen. These interval limits depend on the site-specific N uptake at the respective developmental stage in conjunction with subsequent N-fertilization. Thus, at late developmental stages and high-yielding sites with N-fertilization adjusted for high N uptake allow wider interval limits. The study concluded that at the early stages of stem elongation a ± 10 kg N uptake ha^{-1} interval can be a reasonable choice. Generally, this study observed that a ± 15 kg N uptake ha^{-1} interval is the smallest one feasible for N-fertilization relevant growth stages up to BBCH 50 if a probability of at least 80 % of the data points should be within the interval. These selected error limits ($\hat{y}i \pm 10$ and ± 15 kg N uptake ha^{-1}) are within an acceptable range, if other potential sources of error in N-fertilization, such as distribution accuracy, amount applied, and small-scale crop variability was considered. N-fertilization recommendations based on spectral detecting should not be solely evaluated on the R^2.

For the spectral detection of N uptake in wheat, an unexplained scatter was determined in the models. On the one hand, the destructively obtained N content values were determined as the mean of the entire plant, which cannot be fully spectrally detected due to the vertical gradients in the nitrogen content of the plants (LI ET AL., 2013). Additionally, the spectral value of the plot represents an average value of strongly scattered individual values, and the reference area of the destructively collected data represents a further potential significant source of error.

5.7 Comparison of sensor platforms assessing N uptake of wheat

In Section *II*, a ground-based vehicle (Phenotrac IV), and a UAV equipped with a multispectral sensor were deployed. The UAV could capture the N uptake of wheat comparatively slightly better at BBCH 37 whereas the Phenotrac IV performed slightly better at BBCH 61 but the differences were small.

A main difference between the sensors concerns the bandwidths. Therefore, the NDVI of the Phenotrac IV was calculated with the same bandwidths as used for the UAV NDVI, resulting in no differences in sensitivity. A possible influence of the soil could also be ruled out because the index SAVI (HUETE, 1988) showed no improvement in sensitivity. Another difference between the sensors is the measuring distance to the canopy. The Phenotrac IV has a field of view (FOV) of 24° and a distance to the target surface of 0.8 m. Therefore, both nadir and off-nadir recordings of the canopy take place. APARICIO ET AL. (2004) observed an influence of off-nadir measurements on spectral indices due to the relatively higher reflectance in the visible range compared to the near-infrared wavelength range, which in turn is based on the higher influence of the stems. This observation depends further on the leaf area index (LAI). At low LAI values, the reflection in the near-infrared wavelength range is more pronounced and leads to higher NDVI values for off-nadir measurements which could also be observed in this study at BBCH 37. Further, the data indicate higher index values at the same N uptake. This is in line with MISTELE AND SCHMIDHALTER (2010) who observed an increase in the signal intensity for off-nadir measurements due to more biomass in the sensor`s FOV. GNYP ET AL. (2015) reported advantages of off-nadir compared to nadir measurements in detecting N uptake at early and late growth stages of wheat and, also saturation effects for both measurement geometries. In contrast, this study observed no saturation effects for any index probably due to the observed strong reduction in biomass production in the experimental year. However, at the same site, MISTELE ET AL. (2004) observed saturation effects for all indices in assessing N uptake of wheat. ZHENG ET AL. (2018) also determined the advantages of UAV over ground-based spectral measurements for pre-heading stages in detecting the N content of rice whereas GNYP ET AL. (2016) found no difference between ground-based and aerial sensor platforms in detecting N uptake of wheat.

5.8 Sensitivity of spectral indices detecting N uptake of wheat and N-related traits of maize

Regardless of the sensor platform, indices combining the REDEDGE and NIR bands performed best at BBCH 37 and 61 in detecting the N uptake of wheat (Section *II*). This observation is in line with other studies (MISTELE AND SCHMIDHALTER, 2010; ERDLE ET AL., 2011; GNYP ET AL., 2016; PREY AND SCHMIDHALTER, 2019c).

All maize traits could be spectrally detected equally well with the best-performing indices using the GREEN, REDEDGE, and NIR bands. Other studies observed for grain yield the best-performing indices across the growing season as those using band combinations of GREEN, RED, NIR, and MIDINFRARED (OSBORNE ET AL., 2002; MARESMA ET AL., 2016). For grain and aboveground N uptake, indices using the REDEDGE and NIR region have been shown to be more appropriate (MISTELE AND SCHMIDHALTER, 2008a; LI ET AL., 2014; LI ET AL., 2020; BECKER ET AL., 2020). ZHAO ET AL. (2018) reported for the NNI that the best performing indices were using GREEN and REDEDGE bands. Summarized, the GREEN spectral band was important, but especially the REDEDGE, and the NIR bands in detecting the N-related traits of maize. Due to low variation in chlorophyll absorption in a dense canopy, the red region was insensitive (GITELSON, 2004; HATFIELD ET AL., 2008; NGUY-ROBERTSON ET AL., 2012). Spectral indices are influenced by shadow (ZHANG ET AL., 2015b) and soil (HUETE, 1988). Thus, especially concerning the spectral imagery of maize and particularly at early growth stages, THOMPSON AND PUNTEL (2020) reported the benefits of classifying pixels into classes of plant, soil, and shadow. In this study, unsupervised and supervised classification tools of the ArcGIS program (ESRI®, Germany, Version 10.5.0.6491) were used. The results indicated many pixels were assigned to incorrect classes. Also, the SAVI (HUETE, 1988) and OSAVI index (LI ET AL., 2010) were additionally calculated, but they showed no improvement in sensitivity. Therefore, it was assumed that the error due to shadowing and soil is negligible because very low differences in aboveground biomass were observed between the N levels. Further, performing spectral measurements during midday will reduce possible shadow effects across all developmental stages.

5.9 Future aspects concerning agronomic research

Agriculture is facing multiple challenges. The main challenge for the future decades will be to produce sufficient fiber and food for a growing global population at acceptable environmental cost (ROBERTSON AND SWINTON, 2005). Nowadays, the evolution of agriculture steps into Agriculture 4.0 as the fourth evolution in farming technology puts forward four essential requirements: increasing productivity, allocating resources reasonably, avoiding food waste, and adapting to climate change. For this purpose, the employment of current technologies like the Internet of Things, Artificial Intelligence, Big Data, Cloud Computing, Remote Sensing, etc. is used (ZHAI ET AL., 2020). Nevertheless, in terms of future research, these new technologies need especially field data to develop and validate new approaches. Some lab-based approaches exclusively can reach their limits under field conditions (OLFS ET AL., 2005).

Given the complexity of the nitrogen pathways in agricultural ecosystems (*Figure 3*), these domains of research already need a lot of labor-intensive (field) experiments. In this context, many studies can be mentioned (without claiming to be complete) which have dealt with topics such as ammonia volatilization (PACHOLSKI ET AL., 2006; SMITH ET AL., 2007; KHALIL ET AL., 2009; PELSTER ET AL., 2019), nitrous oxide emissions (KAISER AND RUSER, 2000; KHALIL ET AL., 2009; DENG ET AL., 2015; HU ET AL., 2020a), nitrate leaching (HANSEN AND DJURHUUS, 1996; KORSAETH, 2008; ASKEGAARD ET AL., 2011), application of mineral nitrogen fertilizer (BÜCHI ET AL., 2016; MARTÍNEZ ET AL., 2017; HEIL ET AL., 2018: PREY ET AL., 2019a) and organic fertilizer (BOCCHI AND TANO, 1994; SCHRÖDER ET AL., 2006; DE FRANÇA ET AL., 2021;), effect of crop residues (HART ET AL., 1993; MALHI ET AL., 2006; BAKHT ET AL., 2009), tillage systems (MELAJ ET AL., 2003; VETSCH AND RANDALL, 2004; HALVORSON ET AL., 2006), plant N uptake (LUKINA ET AL., 2001; PRESTERL ET AL., 2002; LIAO ET AL., 2004; CIAMPITTI AND VYN, 2011), biological N_2 fixation (CARRANCA ET AL., 1999; COLLINO ET AL., 2015; GOLLNER ET AL., 2019), atmospheric deposition of nitrogen (ANDERSON AND DOWNING, 2006; SUN ET AL., 2018), mineralization of organic nitrogen (APPEL AND MENGEL, 1990; MILLER AND GEISSELER, 2018; CANISARES ET AL., 2021), denitrification (CASTALDELLI ET AL., 2019; FORTE AND FIERRO, 2019; ROHE ET AL., 2021). Also, in terms of spectral sensing, for example, a lot of application-oriented research was necessary, on which this work is also based (ERDLE ET AL., 2013; KIPP ET AL., 2014a; KIPP ET AL., 2014b; BARMEIER AND SCHMIDHALTER, 2016; PREY AND SCHMIDHALTER, 2019d).

As indicated in this work, field experiments face many not controllable environmental conditions (e.g., weather), which in turn makes the outcome uncertain. Further, a lot of site conditions (e.g., different soils) have to be studied, which increases the number of experiments. To meet these requirements, a pool of sufficiently trained and educated researchers and research facilities must be available to run as many (field) experiments as possible. Existing structures at universities, but also vocational schools and further educational institutions should be maintained or expanded which include necessary investments. EVENSON ET AL. (1979) pointed out that science-orientated agricultural research is profitable when associated with technological research and annual rates of return on research expenditure are in the order of 50 percent. Nowadays, one crucial precondition to achieve the big targets of climate neutrality and biodiversity protection is to have sufficient public funding reserved for agricultural research, and models show that every euro spent on research & innovation will return 10 to 11 euros to the economy (HULOT AND HILLER, 2020). Unlike physical capital, knowledge capital has the potential to generate spill-overs, which means applications beyond the locality or application for which it was originally intended (FUGLIE, 2017). However, the supposedly most important point is the social dimension of the issues affecting agriculture, which is indispensable for viable responses to societal challenges related to agriculture (PIRSCHER ET AL., 2021).

Conclusions

The results of **Section *I*** (Heinemann and Schmidhalter, 2021) confirm the usefulness of a simplified reduced soil sampling strategy per field for soil mineral N (nitrate-N + ammonium-N, “N_{min}”) compared to crop-specific, regionally representative N_{min} values offered by the official advisory authorities in wheat and maize. The results were observed for field sizes in the range of 1.0–12.7 ha. An extrapolation to larger-sized fields seems possible but needs to be further investigated. Heterogeneous fields should be sampled site-specific. Furthermore, it is recommended to aggregate single soil layer samples to one total soil sample depth for further analysis. This approach reduces the workload and costs and provides site-specific N_{min} values for further N-fertilizer decisions. The latter could be demonstrated at two locations in wheat. However, the individual soil layers of no-till managed fields should be analyzed separately. The combining of single soil layers is more recommended for the determination of the absolute N-fertilization requirement. Additionally, the findings pointed out that soil mineral N varies yearly and therefore requires therefore annual sampling. The annual soil sampling could not be derived by crop response to simplified soil N_{min} through multispectral satellite imagery (Sentinel-2) and therefore emphasizes the need for soil sampling.

Section *II* (Heinemann et al., 2022) highlights the additional use of agronomic error intervals besides conventional statistics in spectral detection of the N uptake in wheat. The requirement exists because commonly used statistics such as R^2 depend mostly on the growth stage and year effects and further statistics such as RMSE and MAE only average the error which leads to the under- and overestimation of many observations. Generally, models including data of extreme N levels could be biased and these observations should be excluded from further analysis. Furthermore, the results suggest that spectral detection of the N uptake is more influenced by differentiation of the biomass than the N content. As carrier vehicles, UAVs and ground-based systems are equally well suited, and spectral indices combining REDEDGE and NIR bands are the most suitable to detect N uptake in wheat

Section *III* (Heinemann and Schmidhalter, 2022) provides the usefulness of the additional use of agronomic error intervals besides conventional statistics in spectral detection of N-related traits (aboveground and grain N uptake as well as NNI) and grain yield of maize. The requirement is recommended because widely used statistics such as R^2 depend mostly on year effects and the growth stage, and further statistics such as RMSE and MAE only average the error which leads to under- and overestimation of many observations. The defined interval limits are consistent across years and growth stages because most spectral indices are dominated by biomass. The agronomic evaluation should also support ex-ante and/or ex-post analysis of N-fertilization in maize. Across all, UAV-derived spectral indices performed best when GREEN, REDEDGE, and NIR bands were combined.

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