Statistical and In-field Challenges Involved in Quantifying Crop Nitrogen Use Efficiency (NUE) and Spatial Soil Fertility in Central Alberta

by

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Abstract

Modern agriculture faces the conundrum of a looming threat of food scarcity and heightened pressure on natural resources to address and sustain increasing food demand. Improving nutrient use efficiency is crucial to sustainable food production. It can be helpful in tackling this critical challenge while delivering the required benefits on social, environmental, and economic fronts. Given the limited availability of readily accessible available soil nitrogen (N) and the high cost of synthetic nitrogenous fertilizers, nitrogen use efficiency (NUE) becomes central to the effectiveness of any management practice aimed at sustainable agriculture. In this study, I evaluated the statistical challenges involved in defining NUE as a ratio of grain productivity to available soil nitrate (AN). Ratio analyses and different regression models were used to compare NUE. Measures of goodness of fit showed that quadratic regression (QR) models were comparatively more robust in estimating NUE. This finding elucidated a fundamental limitation in most analyses of NUE as a ratio matrix, as it negated the assumption of isometry crucial to validity of the derived conclusions. Nonetheless, results from QR analysis can be extrapolated to extract information of practical significance, such as the agronomically optimum N rate (AONR) and economic optimum N rate (EONR). Moreover, sample size calculations elucidated the need for a large number of plots to distinguish genotypes differing for NUE; therefore, imposing a logistic constraint to accurately assess differences in NUE.

Strategies for improving nutrient management in croplands such as the 4R Nutrient Stewardship offer a promising avenue to address the seemingly contrasting goals of modern agriculture. In this study, I compared multiple linear regression, a non-geostatistical technique, to different geo-statistical techniques, including ordinary kriging (OK), ordinary cokriging (OCK), and regression kriging (RK) to decipher the spatial structure of soil fertility parameters. Based on cross-validation

estimates, OK in most cases proved to be the model choice to predict soil nutrients, including available nitrogen, readily available phosphorus, and available potassium. In contrast, RK was the best performing method to estimate cation exchange capacity, pH, and organic matter. Landscape position did not show a strong spatial correlation with soil fertility parameters and grain productivity, as terrain attributes failed to substantively improve the corresponding predicted estimates.

Dedication

This thesis is the culmination of un-wavering support from my family. To Ami and Abu, I am eternally grateful for all your advice, support and prayers. I know, it might sound cliché, but I owe everything to you two. Your grit, wisdom, tenacity and humbleness are truly admirable, and have kept me inspired during this endeavor. To my beloved siblings, Sarmad and Rohma, your uplifting messages (and cat memes!) have been a source of comfort and joy. To Nani, my ever-loving cuddly grandma, thank you for all the un-conditional love. Last but not least, to Phupho, I wish you were still around to applaud and cherish our small achievements. You are dearly missed!

This is for all of you!

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Abbreviations

AE	agronomic efficiency
AIC	Akaike's Information Criterion
AK	readily available potassium
AN	available soil nitrate
AnP	annual precipitation
AONR	agronomically optimum N rate
AP	readily available phosphorus
AR	apparent recovery
B	boron
BMP	best management practices
CEC	cation exchange capacity
CIMMYT	Centro Internacional de Mejoramiento de Maíz y Trigo (also known as International Maize and Wheat Improvement Centre in Mexico)
cm	centimetre
Cu	copper
CV	coefficient of variation
CV_{sill}	coefficient of variation sill
D	level of accuracy
d.w.	dry weight

EONR	economic optimum N rate
Fe	iron
G	grams
G_w	grain yield
G_{wf}	grain weight with N application
G_{wo}	grain weight without N application
GPS	global positioning systems
ha	hectare
IN	inorganic nitrogen (NO_3–N and NH_4–N)
kg ha^{-1}	kilogram per hectare
KS	Kolmogorov-Smirnov
lb ac^{-1}	pound per acre
LIDAR	light detection and ranging
LR	linear regression
M	metres
MA	major axis
MAE	mean absolute error
meq	milliequivalent
Mg	magnesium
Mg	milligram
Mn	manganese
MLR	multiple linear regression
Mm	millimetre

MSE	mean square error
Mt	million tonnes
N	nitrogen
N	sample size
N_f	nitrogen uptake with nitrogen application
N_o	nitrogen uptake without nitrogen application
NO_3–N	soil nitrate
N_s	nitrogen supply (amount fertilizer or/and available soil nitrogen)
N/S	not specified
NSR	nugget to sill ratio
N_t	total nitrogen in plants
NUE	nitrogen use efficiency
NUpE	uptake efficiency
OCK	ordinary cokriging
OK	ordinary kriging
OLS	ordinary least square
OM	organic matter
PA	precision agriculture
PE	physiological efficiency
PFP	partial factor productivity
ppm	parts per million
PWR	piecewise regression

Q-Q	quantile-quantile
QR	quadratic regression
R^2	coefficient of determination
RCBD	randomized complete block design
RK	regression kriging
RMA	ranged major axis
RMSE	root mean square error
$RMSE_d$	root mean square error standardized
$RMSE_n$	normalized root mean square error
SIM	spatial interpolation method
SMA	standard major axis
T	t statistic
t_0	threshold
TN	total soil nitrogen
UE	utilization efficiency
USDA	U.S. Department of Agriculture
VR	variable rate
VIF	variance inflation factor
Z_{crit}	Z critical
Z_{pwr}	Z power
Zn	zinc

Symbols

α	alpha

β	power
β_0	intercept
β_1	slope
$\hat{\sigma}$	prediction standard error
σ^2	variance
$\boldsymbol{\varepsilon_0}$	error
r	pearson correlation coefficient
λ_i , $a_{i,,}$ b_i	kriging weights assigned to the measured value
λ_i e(Z_i)	residual for a given variable at location i
γ(h)	semivariance for sampling pairs separated by distance h
°C	degree Celsius
$C_o + C$	semivariogram sill
H	distance between sampling pairs
$\overline{X}$	mean for a given variable
x	regressor
$\hat{y}$	predicated value of a variable
Z	measured value for a given variable
$\hat{Z}$	predicted value for a variable

Chapter 1: Introduction

1.1. The Green Revolution

One of the most significant changes in agricultural productivity during recent history was the green revolution. It refers to a period of technological and agronomic advancements that have helped to sustain the growing world population by development of input-responsive, high yielding varieties of wheat and rice (Khush 1999; Khush 2001). Two major advancements that led to the advent of green revolution are development of the Haber-Bosch process (Galloway *et al.,* 2013), and introduction of dwarfing genes in major crops (Evenson and Gollin 2003).

Identification of dwarfing phenotypes during the early 20th century started this revolution. Dwarfing genes, though largely unknown at the time, came from a Japanese semi-dwarf wheat variety, Norin 10 (Reitz and Salmon 1968). These dwarfing genes were bred into commercial wheat varieties as part of breeding programs in U.S. Department of Agriculture (USDA) and Centro Internacional de Mejoramiento de Maíz y Trigo (CIMMYT, also known as International Maize and Wheat Improvement Centre in Mexico). The wheat dwarfing genes (reduced height; *Rht*) were later identified as *Rht-B1b* (formally known as *Rht1*), and *Rht-D1b* (formally known as *Rht2*) genes (Hedden 2003; Borojevic and Borojevic 2005). These genes repress gibberellin responsive growth, and result in reduced stem elongation. As a result, lodging associated yield losses are significantly reduced (Peng *et al.,* 1999; Saville *et al.,* 2012). Moreover, these phenotypes have a higher dry matter harvest index, as they allow the plants to allocate more resources towards grain (Rebetzke *et al.,* 2012).

1.1.1. Environmental Consequences of Green Revolution-Induced Agricultural Intensification

Between 1969-2017, wheat and rice productivity has increased by 213% and 148%, respectively (FAO STAT, 2018). This increase in grain productivity was achieved through the development of high-yielding varieties which require high inputs, in particular a higher nitrogen (N) supply (Figure 1.1). However, N is a limiting nutrient in most cropping systems. Production of synthetic, N-rich fertilizers through the Haber Bosch process has addressed this limitation by making available a large amount of reactive N as fertilizers (Erisman *et al.,* 2008). This agricultural intensification has included a shift in cropping systems from polyculture to a monoculture system (Tscharntke *et al.,* 2005). This change in dynamics of cropping pattern and cultivation intensity has led to several environment issues with local, regional and global consequences (Altieri and Nicholls 2017).

Local environmental effects include detrimental impact on soil health, including loss of soil through soil erosion and a decline in biodiversity (Tilman *et al.,* 2001; Foley *et al.,* 2011). Maintenance of intensively managed cropping systems through application of large amounts of N-rich fertilizers, and different agronomic practices affects physical and biological soil properties (Matson *et al.,* 1997). These agricultural practices not only deplete soil resources, but also affect the ability of soil to sustain biogeochemical processes, such as the N cycle; (Barrios 2007; Postma-Blaauw *et al.,* 2010; Tsiafouli *et al.,* 2015; Bender *et al.,* 2016). Consequently, the dwindling N pool is further depleted.

To offset the limited availability of biologically active N, more synthetic N fertilizers are added, and this perturbs the natural N cycle (Galloway *et al.,* 2004; Gruber and Galloway 2008; Ward 2012; Fowler *et al.,* 2013). Moreover, the asynchrony between time of N application, and plant demand further exacerbates the imbalance between various N fluxes (Cassman *et al.,* 2002;

De Oliveira *et al.,* 2018). According to some estimates, plants are only able to use 30-50% of applied N (Tilman *et al.,* 2002). The remaining is lost from the soil through leaching, surface run-off, denitrification, and volatilization (Fowler *et al.,* 2013). Besides economic losses, this loss of N also results in environmental hazards that have regional implications.

One example is the degradation of aquatic ecosystems through anthropogenic enrichment with excessive N. Leached N, primarily NO_3-N, percolates through the soil profile to a region below the root zone, where it is not only unavailable to plants (Cameron *et al.,* 2013), but also has a high propensity to enter the groundwater reservoirs (Vitousek *et al.,* 2009). Deposition of this N rich water into the aquatic ecosystem causes prolific growth of algae and phytoplankton, which limits light availability (Diaz and Rosenberg 2008), and causes the death of aquatic fauna and flora. Subsequent microbial decomposition creates an anoxic micro-environment which is known as "dead zone" (Chislock *et al.,* 2013). This phenomenon of profuse growth in response to increased availability of a limiting nutrient is known as eutrophication. Interacting local and regional environmental consequences trigger a suite of reactions that affect the properties of an ecosystem at a global scale. The environmental effects of high-intensity agriculture are expected to worsen because few scientific studies foreshadow a failure in long-term sustainability of these agronomic practices (Tilman *et al.,* 2011).

1.2. Need of Nitrogen Use Efficiency (NUE) in Crop Plants

The human population is expected to increase to 9.1 billion by 2050 (FAO, 2015). To sustain this growing population, there will be a need to increase food production. According to FAO, food production should increase by 70% to fulfill population's dietary requirements (FAO, 2009). This scenario increases the pressure on land and water resources which are fundamental units of the food production system.

In most cropping systems, biologically fixed N is insufficient to completely fulfill plants' needs for different growth and developmental processes (Beatty and Good 2011). This limited availability of N often leads farmers to overfertilize their fields with excess amounts of N (Diacono *et al.,* 2013). This reliance on large amount of nitrogenous fertilizers is environmentally hazardous, and has resulted in serious perturbation of the global nitrogen cycle (Fowler *et al.,* 2013). This progressively deteriorating situation has prompted the goal of developing fertilizer-efficient crop plants. It has also resulted in a change of target goals, from increased food production to sustainable food production, and has placed premium on improving Nitrogen Use Efficiency (NUE) of cropping systems (Hirel *et al.,* 2011; Hawkesford 2014).

1.2.1. Definitions of NUE

Nitrogen is the most important, and expensive crop nutrient to be applied. Therefore, NUE is crucial for farmers to maximize their returns (Parry and Hawkesford 2010). However, complex environmental interactions make NUE a difficult trait to measure (Sharma and Bali 2017). Nitrogen use efficiency is a key concept in sustainable agriculture, and has been the subject of rigorous research and recent literature. However, NUE breeding programs are still in their nascent stages due to the inherent complexity of this trait. Furthermore, the inability to accurately assess NUE further limits the scope of these breeding programs.

Definitions of NUE have changed over the course of time, and there is no universally accepted way of defining this trait. In most cases, NUE is defined according to the background of the researchers e.g., soil scientists define it in terms of plants' efficiency to uptake added or available soil N, while physiologists define it in relation to the efficiency of plants to remobilize and assimilate the absorbed N into grain yield. There are several definitions of NUE available in the scientific literature (Table 1.1), and each term carries a different meaning in different contexts (Weih *et al.,* 2011). The most commonly used definition of NUE is the efficiency of uptake of applied or available N from soil, and is defined as a *ratio* of grain productivity to available or supplied N. However, there are a number of inherent statistical issues revolving around the use of this definition. These statistical issues along with in-field challenges involved in accurate assessment of NUE are described in detail in Chapter 2.

1.3. Approaches for Improving NUE in plants

1.3.1. Genetics Based Approaches for Improving NUE in Plants

High genetic variability has been reported for NUE and NUE related traits in wheat, barley, rice, maize, canola, and many other crops (Monostori *et al.,* 2017). Moreover, deciphering the molecular basis of NUE shows that it is a polygenic trait that is orchestrated by multiple genes controlling different biochemical, physiological, and morphological functions (McAllister *et al.,* 2012). Access to different tools for genome sequencing has generated copious amount of genotypic data. Over the last decade, a large number of N-responsive genes expressed at different N levels, and stages of N metabolism have been identified (Bi *et al.,* 2009). This body of knowledge suggests that conventional breeding and transgenics offer a plausible avenue for improving NUE. However, this approach is not as simple as it seems, and this technology is still in developmental stages. Moreover, several extrinsic factors limit the success of developed varieties during the field evaluation. Variation due to genotype x environment interaction is profound (Senthilvel *et al.,* 2008), and may be as large as genotypic variations (Han *et al.,* 2015). Moreover, soil N supply is spatially and temporally variable. This labile N variability reduces the reproducibility of NUE indices over multiple years (Dobermann 2005). The interactive effect of N availability with other cropping variables, such as availability of water and other nutrients, also affects the accurate assessment of NUE (Dobermann 2005). In addition, the prevalence of different definitions of NUE, and different cropping practices makes it difficult to compare available studies across different environments and years.

1.3.2. Management Based Approach for Improving NUE

Best Management Practices (BMPs) have been highlighted as a sustainable solution to curb N losses (Bruulsema *et al.,* 2008). Best Management Practices exploit different components of cropping systems, such as water, nutrient, and farm management practices (e.g., tillage) to optimize the efficiency of the production unit while maintaining profitable returns, and minimizing environmental hazards (Mikkelsen 2011). The same concept of BMPs has been applied to fertilizer management, an approach known as 4R nutrient stewardship. It is a relatively simple framework consisting of four components that are inter-related; right rate, right time, right place, and right source (Table 1.2). The success of this approach depends on a sound technical knowledge of the underlying principles, and the right combination of these components (Bruulsema *et al.,* 2009).

Each of these four components are of interest to different stakeholders who tailor a basic framework for given field conditions, such as soil properties, weather conditions, and available farm management resources (Johnston and Bruulsema 2014). Stakeholders including farmers, research institutions, government institutions, and the public have different objectives and performance parameters (Table 1.3) to evaluate the efficacy of the adopted operations. However, the ultimate goal of economic and environmental sustainability is consistent between different stakeholders.

1.3.2.1. Right Rate and Right Place for Fertilizer Application

Fertilizer cost is an important consideration for the farmers in gauging economic returns. This makes application of the right rate of fertilizer at the right place a key element that forges successful implementation of the 4R framework. Theoretically, it is a simple concept that implies that added nutrients are sufficient to fulfill plant's nutrient requirement at a given place, and the intended economic, social and environmental goals are also achieved. However, there are a few factors including inherent soil properties, weather and climatic conditions that govern this decision of N application (Mikkelsen 2011).

1.3.2.2. Factors Affecting Right Rate and Right Place of Fertilizer Application: Spatial Soil Variability

Soil is a dynamic natural resource that is quite heterogeneous in its properties. There are two important classes of soil heterogeneity; lithological and inherent soil heterogeneity. Lithological heterogeneity is the distribution of different lithological layers in a soil matrix. Inherent soil heterogeneity deals with the distribution of soil properties across a continuum of the soil profile (Phoon and Kulhawy 1999; Elkateb *et al.,* 2003). This type of soil heterogeneity is due to interaction of different permanent features (such as, soil type and topography), and variable features (such as, cropping and management history and weather conditions) of the landscape (Lobb 2011; Diacono *et al.,* 2013). Characterization of inherent soil variability is complex due to the interaction of cumulative factors at different spatial and temporal scales (Zhang *et al.,* 2011). Many studies on soil variability encompass a combination of these varying factors. For example, soil N heterogeneity across a landscape is not explained by a single factor, but is in fact, a result of interaction of these variable soil and environmental interactions. The interactive nature of these factors should be taken into consideration while deducing practical implications for field management decisions.

Among landscape features, soil type and topography are the two most important determinants of soil variability. Variation in soil types not only affect the availability, but also the retention of water and nutrients in the soil (Tola *et al.,* 2017). Topography has a strong correlation with spatial variability of different soil properties, both physical and chemical (Ceddia *et al.,* 2009). It affects the physical movement of soil, that in turn, affects the spatial distribution of soil nutrients and soil moisture across the landscape (Noorbakhsh *et al.,* 2008; Noorbakhsh *et al.,* 2011). Soil run off from hilltops deposits nutrient rich topsoil to low lying areas, hence eroded hilltops can be less fertile. This downwards movement of soil leads to the accumulation of nutrients, and soil organic matter in foot slope positions (Balasundram *et al.,* 2006). However, accumulation of soil moisture in low-lying depressions can also lead to nutrient loses (Moulin *et al.,* 1994). Difference in soil fertility profile can also affects soil quality, thus reducing crop growth and productivity in high positions (Verity and Anderson 1990). However, the degree and nature of such variability that is changing as a function of landscape position, is poorly understood.

In addition to these permanent landscape features, variable features such as temporal variability of precipitation, also interplay with patterns of spatial soil variability (Santillano-Cázares *et al.,* 2012). Moreover, different agricultural practices such as conventional tillage and cropping patterns, also affect inherent soil variability by changing physical and chemical soil properties. These changes in soil properties affect the ability of soil to sustain biological functions (such as nutrient cycling) by altering soil microbial biomass and activity (Spedding *et al.,* 2004; Bausenwein *et al.,* 2008; Lauber *et al.,* 2013).

1.3.2.3. Approaches to Assess Soil Variability

Since its introduction in the early 1990s, yield monitoring has become common in modern agriculture (Stafford *et al.,* 1996). It is defined as a process of gathering and processing geo-referenced data for different crop characteristics, such as crop yield and soil moisture. A basic crop yield monitoring system comprises of a range of different sensors used for different purposes (Adamchuk *et al.,* 2008). Software is used to extract and process raw data collected from these sensors. Data processing, and sensor calibrations are crucial for developing accurate yield maps. Sensors are calibrated according to the vendor's operation manual to ensure accuracy of the collected raw data, which is then subjected to post-processing cleaning to identify and address commonly measured physical errors, such as erroneous travel distance and flow delay measurements, errors in header position sensor, and header cut-width (Luck and Fulton 2014; Luck and Fulton 2015).

Crop yield monitoring serves as a tool to make educated decisions for managing in-field variability to optimize economic and environmental benefits. At the same time, it offers a good starting point for building an information repository to assess soil variability (Zhang *et al.,* 2002). In preliminary analyses, the in-field grain yield variation could be used as a proxy for the soil variability. Grain yield maps from multiple years help to identify areas of consistent low and high productivity; however, they do not identify the underlying causes explaining this yield variability (Johnson *et al.,* 2003). Therefore, this information can be of limited use to the farmers unless productivity-limiting factors are interrogated through soil sample analysis (Diacono *et al.,* 2013).

1.3.2.4. Soil Sampling and Analysis as a Tool to Explain Causes of In-field Yield Variability

In the wake of growing environmental and economic concerns, optimum nutrient management is of paramount importance. Soil sampling and analysis are crucial for developing soil fertility profiles that form the basis for nutrient management operations (Carter and Gregorich 2006). However, the success of these operations depends on the accuracy of soil analysis. Therefore, it is important to collect and analyze soil samples that are true representatives of the field conditions. A well-designed sampling plan serves as a guiding principle in accurate assessment of soil nutrient status. Sampling depth, intensity, time, and location are the main components of a sampling plan that ensures soil samples are collected at appropriate time, and depth with an adequate spatial density (Carter and Gregorich 2006). Moreover, a host of other factors, such as cropping history and laboratory costs are also taken into consideration while developing a sampling plan.

As a part of a sampling plan, selection of appropriate sampling strategy is also critical to develop accurate soil maps. Different sampling strategies, such as random composite, directed random composite, benchmark, landscape-directed benchmark, and grid sampling can be used depending on resources, field assessment, and the amount of information needed. This baseline information is not only useful for the farmers to manage the causes of in-field yield variability by using modern agronomic approaches, such as variable rate fertilizer application (Iqbal *et al.,* 2005), but also provides important repository information that serves as a blueprint for developing sampling plans for modelling environmental and agricultural management systems (Jones *et al.,* 2017).

1.3.2.5. Heterogeneity in Soil Variability

Among other macro-nutrients, soil N exhibits high variability (Table 1.4) at both spatial and temporal scales. This variability becomes a nuisance to site-specific management intended to reduce N footprint on the environment. Studies have been conducted to document spatiotemporal variability of soil N (Robertson 1988; Cain *et al.,* 1999; Stark *et al.,* 2004; Huang *et al.,* 2007; Wang *et al.,* 2007). Variability in soil N could be structured at a much finer scale, and it could vary at scales as small as 1 m (Robertson 1988). According to geostatistical analysis conducted by Robertson 1988, nugget variance (i.e., variance for a given variable of interest at a scale smaller than minimum sampling distance) accounted for 20% of the total sill variance (maximum variance between spatially auto-correlated sampling pairs), indicating that some variability in soil N could be spatially structured at a scale less than 1 m, whereas another study conducted by Wang *et al.,* 2007 showed 32% of the total variability in soil N could be operating at an interval of less than 5 m. Even though such small-scale variability is logistically inviable to sample and manage, it should still be recognized since site-specific management is incumbent on knowledge of the scale at which this variability operates.

1.3.2.6. Limitation of Soil Sampling and Analysis

Micro-managing the in-field yield variability requires a comprehensive dataset of spatial soil variability. However, in most cases, due to financial and practical reasons, collected soil data is of inadequate density, and this sparsity of soil information data becomes a major bottleneck in its application in precision agriculture (PA) (Oliver 2010). Geostatistics offers a solution to alleviate this limitation by interpolating data values for unsampled locations based on information collected from the sampled locations.

1.4. Geostatistics—A Solution to Sparse Data

Geostatistics is a branch of statistics used to develop mathematical models to characterize spatial and spatiotemporal phenomena. Originally developed for assessment of mining sites, geostatistics is now finding widespread applications in ecological, environmental, and agricultural studies (Zhou *et al.,* 2007). It is used to analyze geo-referenced datasets to decipher the underlying spatial patterns by exploiting spatial autocorrelation between the data points (Li and Heap 2014). The model outcome is a map showing continuous surface explaining the intrinsic spatial nature of variable(s) being modeled by assigning a definitive value at each given point (Johnston *et al.,* 2001). The developed map is checked to ensure that the interpolated values, and other model parameters, such as associated measures of uncertainty, are rational. If needed, necessary adjustments are made, and the resulting model can be used in making informed management decisions (Johnston *et al.,* 2001).

Geostatistics is based on Waldo Tobler's First Law of Geography, "Everything is related to everything else, but near things are more related than distant things" (Miller 2004). According to the foundational principle of geostatistics, there is a degree of continuity in the spatial configuration of the regionalized variable. Variation of soil attributes in space is not random, but is in fact, structured in a way that this degree of variability decreases as the distance between the two sampling points decreases (Seidel and de Oliveira 2016).

1.5. Application of Spatial Soil Information in Precision Agriculture

Precision agriculture (PA; also known as site-specific agriculture), is defined as a set of agronomic practices that can contribute to a viable solution for sustainable food production. The concept of PA has been around for decades. It is based on an intuitive idea of tailoring different inputs contingent on spatial and temporal soil and crop requirements. There are two major advantages of using these PA practices: (1) the preservation and improvement of environment by limiting different sources of environmental pollution, and (2) increased economic returns owing to reduced input cost (Diacono *et al.,* 2013).

Precision agriculture is a three-tiered approach; consisting of assessment of in-field variability, followed by management of this variability, and finally, evaluating the efficiency of the applied field operations (Figure 1.2). Accurate assessment of in-field soil variability is crucial for the overall success of this approach. Therefore, it is important to understand the underlying causes contributing to such variability.

Although PA technology became available in the mid-1980s in Western Europe, Australia, Canada and USA adoption of this technology has been geographically and temporally variable (Swinton and Lowenberg-Deboer 2001; Micheels and Nolan 2016). This uneven adoption of PA technology is tied to a number of factors, such as land and labor availability, initial investment cost, public awareness about environmental hazards of intensive farming and stringency of environmental legislations. Moreover, adoption of leading application of PA depends upon the regional priorities, for example, mitigating detrimental effects of intensive farming is the focal point for PA adoption in Europe.

Yield monitoring and nutrient management are the two leading applications of PA. In Canada, 5-15% of the land under cereal production uses either one or a combination of these technologies (Swinton and Lowenberg-Deboer 2001). Being a land-abundant country, Canada offers feasible conditions for the assimilation of PA technology; however, a large number of farmers in Western Canada still hesitate to adopt these technologies due to the lack of supporting evidence of environmental and economic gains of making this transition. Research on quantification of spatial heterogeneity of soil properties using geostatistics is lagging in Western Canada. Recently, the effects of controlled traffic farming (a form of PA operation) on soil properties were quantified in the Canadian prairies, using geostatistical modelling (Guenette and Hernandez-Ramirez 2018). According to this study, geostatistical methods performed better than non-geostatistical methods to capture the underlying spatial structure of soil properties.

1.6. Goals of this thesis

Site-specific management relies on accurate quantification of soil fertility parameters. However, there is a large knowledge gap in quantification and mapping of these soil fertility parameters to gauge the extent of spatial heterogeneity within a field. Moreover, there are limitations in the accurate assessment of NUE. On one hand, it is a difficult trait to measure, and on the other hand, these measurements are also subjected to different statistical and in-field challenges. The purpose of this thesis is to bridge this knowledge gap. Specific research objectives of this thesis included:

1. The investigation of statistical challenges involved in defining NUE as a ratio of grain productivity and available soil nitrate through comparison of different statistical models.
2. The determination of in-field variability in soil fertility parameters through comparison of different geostatistical methods.

1.7. Figures and Tables

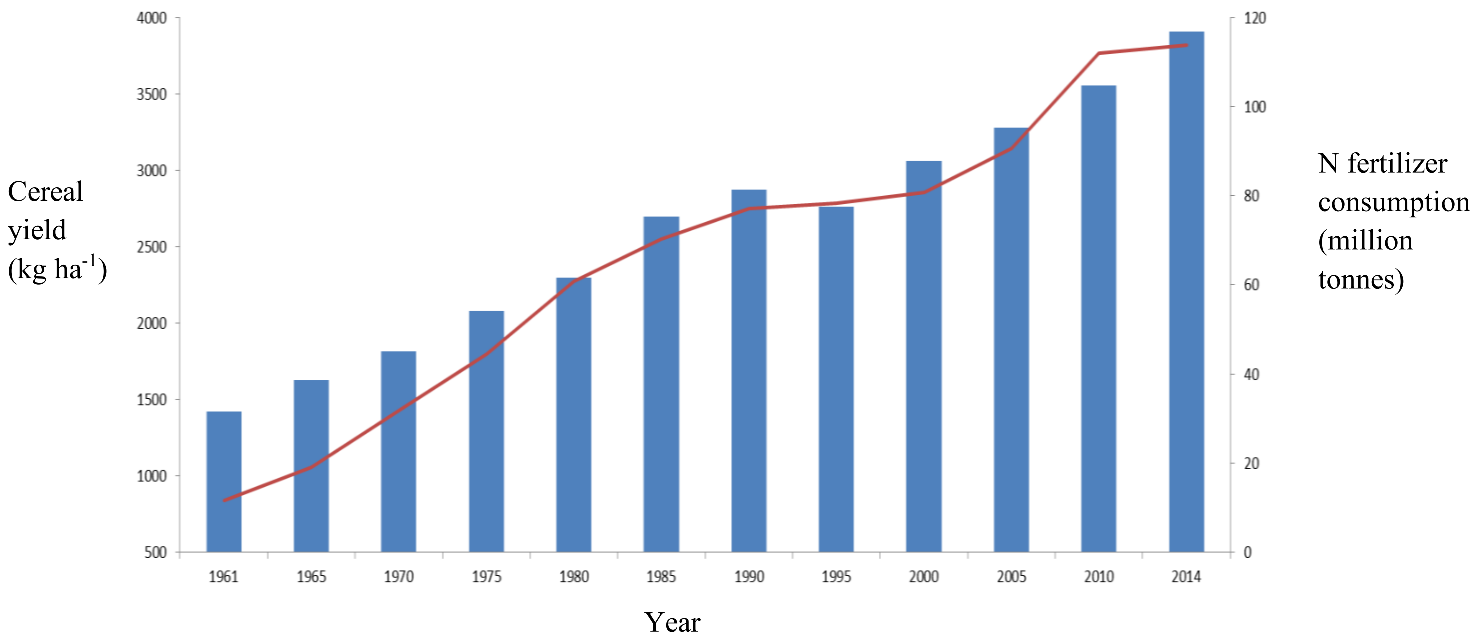

Figure 1.1. Global yield and fertilizer consumption trends from 1961 to 2014. Line graph shows an increase in consumption of nitrogenous fertilizers from 12 Mt in 1961 to 114 Mt in 2014, and is expected to increase by approximately 2% annually. Cereal yield (including wheat, rice, maize, sorghum, oats, barley, millet, rye, soybean), shown by bar graph, increased by 175% from 1961 to 2014. Data Source: Fertilizer (FAOSTAT) (accessed December 2017)

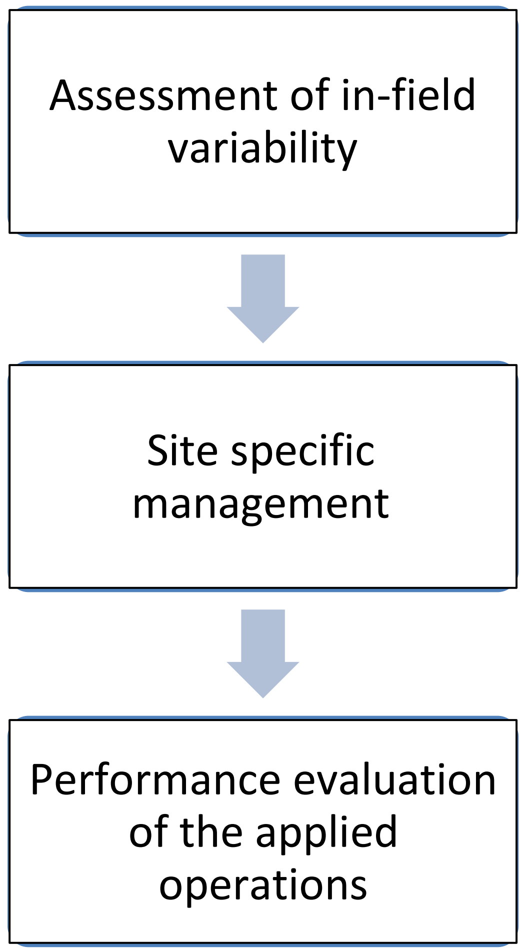

Figure 1.2. Schematic representation of the basic components of precision agriculture.

Table 1.1. Common measures of Nitrogen Use Efficiency (NUE). All of these indices differ slightly in terms of measures taken into consideration during these calculations. Nonetheless, they capture the same essence of NUE, i.e., plants' ability to assimilate and remobilize N (soil N supply and/or added N fertilizer) into the final product–grain yield. Using these indices for assessment of NUE requires careful analysis of the research objectives, and use of these estimates depends on the crop, harvest product, and research objectives (Adapted from Dobermann 2007).

Measure	**Formula***	**Applications**	**Limitations**
Partial factor productivity	PFP= G_w/N_s	It is the most commonly used NUE term, and is a good indicator of long-term trends.	It is of limited spatial scale, and there is a difficulty in making comparisons between different crops and cropping systems across different geographic regions. It is also subjected to several statistical limitations.
Uptake efficiency (also known as partial nutrient balance)	NUpE= N_t/N_s	It is based on the expression of efficiency (i.e., ratio of output to input). Typically, it is used to answer: "How much N has been	This measure of NUE provides misleading information of soil fertility profile, as all N inputs (such as biosolids, biologically

		allocated to the grain in comparison to the amount of N supplied?"	fixed N, residual N etc.), and outputs (N loss through soil erosion, and leaching) are rarely added in the calculations.
Utilization efficiency (UE)	UE= G_w/N_t	It is used in breeding programs to assess performance of genotypes.	Different biotic and abiotic stresses skew this measurement.
Physiological efficiency (PE)	PE= $(G_{wf} - G_{wo})/(N_f$ uptake-N_o uptake)	It is used to study short-term field trends.	This measurement requires implementation of a control plot (i.e., a plot without N application) at the site, and farmers are mostly hesitant to include this control plot at their farms. It is not a good measure of long-term field trend, as in the long run, soil N pool gets depleted, hence widening the response between treatment and control plot, and eventually

			resulting in incorrect interpretations of NUE estimates.
Agronomic efficiency (AE)	AE= $(G_{wf} - G_{wo})/N_t$	It reflects per unit increase in yield in response to added N fertilizers, and is used for analysis of economic returns.	Similar to PE, it also requires control plot for accurate assessment of NUE.
Apparent recovery (AR)	AR= N_f uptake - N_o uptake	It expresses crop response to N fertilizer, and reflects the efficiency of cropping system, and management practices by indicating potential N losses.	It is subjected to the same limitations as PE and AE.

*G_w = Grain yield, N_s = N supply (amount of fertilizer or/and available soil N), N_t = total N in plants, G_{wf} = Grain weight with N application, G_{wo} = Grain weight without N application, N_f uptake = N uptake with N application, N_o uptake = N uptake without N application.

Table 1.2. Framework for the 4R Nutrient Stewardship. Combinations of different agronomic practices are used to achieve the larger goal of sustainability (Adapted from Bruulsema *et al.,* 2009).

4R Framework	**Scientific principles**	**Important considerations**	**Practices used**
Right rate	Synchronization of nutrient application rate to crop requirement so yield and quality goals are met	Rate of nutrient turn-over from organic fertilizers	Pre-plant fertilization, and in-season adjustments accounting for environmental variables and equipment availability for variable rate application
Right time	Synchronization of soil supply rate to nutrient requirement for critical growth stages	Critical growth stages, logistics of farm operations, and physical soil properties	Pre-plant and split fertilization, foliar application, application of controlled-release fertilizers, and fertilizer additives (urease or/and nitrification inhibitors)
Right source	Complementing fertilizer source to crop requirement	Soil physical properties, equipment availability, fertilizer cost	Granular and liquid fertilizers
Right place	Accessibility of nutrients to plant roots	Soil physical properties, logistics of farm operations, and crop root growth patterns	Banding, and broadcasting injection into the soil

Table 1.3. Performance indicators of the 4R framework. These measures are used to establish the efficacy of the adopted framework for nutrient management. This evaluation scheme is developed by the input of various stakeholders, and their relative importance changes accordingly (Adapted from Bruulsema *et al.,* 2008).

Main idea	Components	Management goals	Performance indicators
Sustainable development	Economic	Productivity	Yield and yield stability
			Quality
		Profitability	Farm income
			Economic returns
	Social	Sustainability of cropping system	Adoption of the applied practices
			Working conditions
			Accessibility to affordable food
			Ecosystems service
	Environmental	Protection against environmental degradation	Soil productivity
			Biodiversity
			Nutrient use efficiency
			Nutrient budget

	Land and water use efficiency
	Water and air quality
	Soil erosion

Table 1.4. Descriptive statistics of studies conducted on variability in soil nitrogen.

N form	**Mean**	**Standard deviation**	**CV (%)**	**Reference**
IN	59.05 ($\mu g\ g^{-1}$ d.w.)	3.30 ($\mu g\ g^{-1}$ d.w.)	5.58	Costa *et al.,* 2015
N/S	2.37 $g\ kg^{-1}$	0.72 $g\ kg^{-1}$	30.38	Guan *et al.,* 2017
TN	0.21 $g\ kg^{-1}$	N/A	10.43	Wang *et al.,* 2015
TN	25 $g\ kg^{-1}$	N/A	37	Dessureault-Rompré *et al.,* 2015
N/S	0.66%	0.28	42.98	Gallardo and Paramá (2007)
IN	183.1 $kg\ ha^{-1}$	88.1 $kg\ ha^{-1}$	48.1	Vasu *et al.,* 2017
TN	0.378%	0.17%	44.73	Wang *et al.,* 2009
TN	1.89 $g\ kg^{-1}$	0.64 $g\ kg^{-1}$	33.86	Xing-Yi *et al.,* 2007
AN	24 $kg\ ha^{-1}$	N/A	39	Shahandeh *et al.,* 2011
AN	8.40 $\mu g\ g^{-1}$	6.57 $\mu g\ g^{-1}$	77.39	Wang *et al.,* 2007
AN	3.36 $mg\ kg^{-1}$	1.60 $mg\ kg^{-1}$	47.62	Redulla *et al.,* 2002

IN: inorganic nitrogen (NO_3–N and NH_4–N); d.w.: dry weight; AN: available soil nitrate; TN: total soil nitrogen; N/S: not specified

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Chapter 2: Approaches and Challenges Involved in Quantifying Plant Nitrogen Use Efficiency (NUE)

2.1. Introduction

Several different approaches are commonly used to estimate nitrogen use efficiency (NUE). The ratio of grain productivity to some measure of nitrogen (N) is the most commonly used definition of NUE (Moll *et al.,* 1982). Ease of application makes ratio analysis prevalent in biological sciences; however, this simple matrix is subjected to numerous limitations that are mostly overlooked while drawing conclusions. Ratio analysis is based on an implicit assumption of an isometric relationship between the two variables of interest, i.e., the slope remains the same, and the regression line explaining this functional relationship passes through the origin (Packard and Boardman 1988). If the assumption of isometry is not satisfied, then the ratio is dependent on some function of the numerator. Therefore, comparing different groups using this approach could be misleading (Raubenheimer 1995). As an example, a yield of 200 Kg for 100 Kg of available N provides the same NUE ratio at 100 Kg for 50 Kg of N; however, a farmer would clearly prefer the former situation.

Insufficient sample size to distinguish two genotypes differing for NUE, poses another in-field challenge in accurate assessment of NUE. Sullivan and Feinn (2012) emphasized the importance of calculating the minimum number of samples required to test a null hypothesis with a sufficient degree of certainty. Calculating the minimum number of samples ensures that the experimental design is powerful enough to detect the given effect size. Effect size is a measure of substantive significance and is defined as the magnitude of difference between population means. Statistical power is defined as the probability of making a type II error. *A priori* power analysis should be conducted to ensure enough samples are included in the experimental design to detect differences that actually exist between the populations. Unfortunately, these analyses are not part of standard practice. Therefore, there is a probability of making a type II error i.e., failure to reject a wrong null hypothesis, in other words, a false negative finding.

The accurate calculation of NUE is not only of economic importance for farmers to help them exploit maximum potential of the crop plants, but also for plant breeders for the proper evaluation of varieties with improved NUE across different experimental designs and agro-climatic conditions (Weih 2014). However, there is a lack of studies investigating different statistical and in-field challenges involved in assessing NUE. This chapter aims to bridge this knowledge gap by: (i) investigating the statistical challenges involved in defining NUE as a ratio of grain productivity and available soil nitrate (AN), (ii) evaluating different regression models to estimate the functional relationship between grain productivity and available soil nitrate as yield response curves, and (iii) estimating the minimum number of samples needed to discriminate populations differing for NUE.

2.2. Materials and Methods

2.2.1. Experiment Sites

For this study, three commercial sites located north of Edmonton in Sturgeon County, Alberta, Canada, were selected. All the sites are predominantly characterized by moderately fine-textured Black Chernozemic soil with an average growing season precipitation of 286 mm, and mean growing season temperature of 2.67 °C. All these sites have been managed through conventional tillage, and are subjected to arable cropping. A crop rotation with wheat (*Triticum aestivum* L.), canola (*Brassica napus* L.), and field pea (*Pisum sativum* L.) is used at the Bert (53°51'13.4"N, 113°14'06.8"W), while a wheat, and canola rotation is used at the Brad (53°51'41.6"N, 113°14'49.3"W) and the Lamoureux (53°50'06.5"N, 113°12'14.5"W) sites (Figure. 2.1). In the rotation at Brad and Lamoureux sites, canola was grown in 2014, and in 2015, it was wheat. In contrast, the Bert site had field peas in 2014 and wheat in 2015. Therefore, only the Bert site had a N fixing crop in 2014. In 2015, variable rate (VR) of urea was applied (Figure 2.2a – Figure 2.2c). In spring 2015, Bert, Brad and Lamoureux sites also received an additional 100 lbs ac^{-1} of urea (46-0-0) to the field through a broadcast application (Table 2.1 – Table 2.3).

2.2.2. Grain Productivity and Soil Data

Wheat grain productivity data were recorded using the Green Star™ 3 yield monitor mounted on a combine harvester during September 2015. Before harvesting, moisture and grain flow sensors were calibrated for the wheat crop. Wet and dry grain volume (kg ha^{-1}) were recorded at different geo-referenced locations.

During early June of 2015, 2 ha sampling grids were defined across the sites and 30 soil samples were taken from each grid using a tractor mounted Auto-Probe™ at a depth of 0-15 cm. Samples collected from each grid were homogenized to get a representative sample, and sub-samples (~ 50 grams) from this homogenized sample were placed in a labelled plastic bags, and stored at 4°C. Soil samples were sent to Midwest Labs for analysis of available soil nitrate (AN), readily available phosphorous (AP), and readily available potassium (AK). The P1 (weak bray) test was used to estimate AP, and neutral ammonium acetate extraction was used to measure AK. Flow injection analysis was used to analyze AN.

2.2.3. Ratio and Statistical Analysis of NUE

Computing NUE as a ratio of grain yield (y, response variable) to AN (x, regressor or predictor variables) (Table 2.4), helped to visualize some of the above-mentioned statistical challenges. All statistical analyses were completed in R software (R core Team, 2017). The relationship between grain yield and AN in wheat was explored using different regression models. Before fitting a linear model, the assumption of normality was checked through Shapiro-Wilks test. A linear regression (LR) model I (ordinary least square, OLS), $\hat{y}_i = \beta_0 + \beta_1 x_1 + \varepsilon_0$, was fitted (Figure 2.3), where β_0, β_1 and ε_0 are the intercept, slope and error term, respectively.

Fit of the model was assessed through diagnostic graphs (Figure 2.4). Normality and homoscedasticity of residuals were also assessed through the Shapiro Wilks and Breuch-Pagan tests, respectively. To account for sampling error in the explanatory variable, LR model II was performed (Figure 2.3) which computes slope using different methods, such as major axis (MA), standard major axis (SMA), and ranged major axis (RMA). Relationship between grain yield and AN was further explored using quadratic (QR) and piecewise regression (PWR) models (Figure 2.5).

2.2.4. Minimum Sample Size

The minimum number of sampling units required to study a certain effect size with a specified statistical power were calculated using the following formula:

$$\mathbf{N = 4\sigma^2 (Z_{crit}+Z_{pwr})^2 / D^2} \qquad \textbf{[2.1]}$$

Where N is the sum of sample sizes for both varieties, σ^2 is the variance, and D is the minimum expected difference between varieties expressed as a percentage. Z power (Z_{pwr}) and Z critical (Z_{crit}) are the statistical power, and significance criterion used for this analysis. I chose conventional Z_{crit} of 0.05. To ensure that the study is flexible enough to accommodate experimental rationale and feasibility pre-requisite of future studies, I selected Z_{pwr} of 0.80.

2.3. Results

2.3.1. Statistical Analysis of NUE

Computing NUE as a ratio of grain yield to AN demonstrated mean yield gain of **102 ± 24.53**, **232 ± 105.68**, and **164 ± 23.31** kg ha^{-1} for every lb ac^{-1} of AN at the Bert, Brad and Lamoureux sites, respectively (Table 2.4). Average NUE values; however, can be misleading if the relationship between grain yield and AN does not pass through the origin or is non-linear in nature.

Both, exploratory data analysis and the Shapiro Wilks test showed that grain yield and AN data for all the sites were normally distributed. Predicting the effect of the independent variable (AN) on the dependent variable (grain yield) using LR model I, $\hat{y}_0 = \beta_0 + \beta_1 x$, gave the following equations:

Bert: $$\hat{y}_a = -87.4 + 107x \quad [2.2]$$

Brad: $$\hat{y}_b = 3314.3 + 62x \quad [2.3]$$

Lamoureux: $$\hat{y}_c = 2590.9 + 78x \quad [2.4]$$

Where, $\hat{y}$ is the predicted value of grain yield. β_0 is the intercept and β_1 is the slope, and they represent the estimated values of grain yield increase when no N and each additional 1 lb ac^{-1} of soil N is available, respectively. At all three sites, there was a significant linear relationship between grain yield and AN with a slope of **107 ± 12.37**, **62 ± 9.51**, and **78 ± 13.95** kg ha^{-1} grain yield per unit AN (lb ac^{-1}) at the Bert, Brad, and Lamoureux sites, respectively.

Linear regression (LR) model I does not take into consideration the measurement error in the predictor variable. However, LR model II addresses this limitation, and accounts for measurement errors. Major axis (MA), standard major axis (SMA), and ranged major axis (RMA) are three different methods used by the lmodel2 function to compute the slope parameter. Assumptions for each of these methods were assessed prior to deciding which method to use. The principal assumption of bivariate normality, which is common to all three methods, was satisfied (p-value = 0.05). Since the two variables were dimensionally heterogeneous and were correlated, SMA was an appropriate model choice. Using this approach showed a grain yield increase of **117**, **74**, and **91** kg ha^{-1} for every lb ac^{-1} of AN at the Bert, Brad, and Lamoreaux sites, respectively. However, for each site, LR I and II yielded insignificant ($p > 0.05$) differences in NUEs.

Plotting the relationship between grain yield and AN as shown by these three different approaches (Figure 2.3) showed that ratio represented the shallowest relationship between the two variables at Bert as shown by the lower average NUE estimate; whereas, it overestimated this functional relationship for the other two sites, as given by higher average values of NUE (Figure 2.3).

The possibility of non-linear relationship was tested by visual inspection of regression diagnostic plots for each site (Figure 2.4). Each residual vs. fitted plot showed some curvature as opposed to a roughly straight line required in order to meet the assumption of linearity of the residuals. Fitted LR models complied with the assumption of normality as shown by quantile-quantile (Q-Q) plots (Figure 2.4) and the Shapiro Wilks test. Assumption of homoscedasticity (homogeneity of variance) was also verified using the Breuch-Pagan test.

This pattern of distribution was further investigated to see if a different model fitted our datasets better compared to the LR models. Using QR analysis to model the functional relationship between the two variables yielded the following equations:

Bert: $$\hat{y}_i = -3524.1 + 325.6x_i - 3.08x_i^2 + \varepsilon_0 \quad [2.5]$$

Brad: $$\hat{y}_j = 2232.7 + 170.1x_j - 2.04x_j^2 + \varepsilon_0 \quad [2.6]$$

Lamoureux: $$\hat{y}_k = -497.9 + 270.2x_k - 2.79x_k^2 + \varepsilon_0 \quad [2.7]$$

Unlike the LR models where slope was constant, and was independent of value of x, the slope in QR analyses changed throughout the regression line for the quadratic functions, and was given by the following first derivatives:

Bert: $$\hat{y}_{i'} = -6.16x_i + 325.6 \quad [2.8]$$

Brad: $$\hat{y}_j' = -4.08x_j + 170.1 \quad [2.9]$$

Lamoureux: $$\hat{y}_k' = -5.58x_k + 270.2 \quad [2.10]$$

Using equation 2.8, 2.9, and 2.10, the amount of AN where grain yield response became zero, was calculated. For a given site, these first derivates represented the best estimate of NUE as they captured the true dynamics of grain response to AN. The summary tables (data not shown) for the quadratic models showed that both linear (x – soil N) and quadratic (x^2 – soil N^2) terms in these models were significant predictors of the functional relationship between the two variables for each site ($p < 0.001$). Therefore, a quadratic approach should have been included while studying this relationship. This conclusion was further supplemented by examining performance indicators such as root mean square error (RMSE), and normalized root mean square error ($RMSE_n$) for each of these models. Piecewise regression (PWR) was also used to study the functional relationship between the two variables, and it was the best performing model with smaller RMSE and $RMSE_n$ of 357 kg ha^{-1} and 2.13% for the Bert, 379 kg ha^{-1} and 1.54% for the

Brad, and 384 kg ha^{-1} and 1.73% for the Lamoureux site. Performance of the QR models was comparable to PWR models, with RMSE and $RMSE_n$ of 347 kg ha^{-1} and 2.14% for the Bert, 437 kg ha^{-1} and 1.83% for the Brad, and 376 kg ha^{-1} and 1.79% for the Lamoureux site. In contrast, LR models showed higher RMSE and $RMSE_n$ of 602 kg ha^{-1} and 3.83% for the Bert, 534 kg ha^{-1} and 2.31% for the Brad, and 415 kg ha^{-1} and 2.07% for the Lamoureux site (Table 2.5).

2.3.2. Minimum Sample Size

To estimate the minimum number of samples required to distinguish the two genotypes differing for their NUE, I conducted a power analysis. Different parameters taken into consideration for this power analysis included: level of significance ($\alpha = 0.05$), effect size (10% difference in NUE), statistical power, and measure of variability (i.e., variance). To detect a difference of 10% in NUE relative to the mean of the check variety, AC Andrew, the minimum number of plots needed for AC Foremost, Plentiful and Harvest were **53**, **969** and **47** plots, respectively (Table 2.6). The large number of samples required to detect a 10% difference in NUE of Plentiful compared to AC Andrew reflected the high variance (CV = 49%) associated with this cultivar/site. However, a decrease in NUE variability in datasets for AC Foremost (CV = 24%), and Harvest (CV = 14%) corresponded with smaller sample sizes and lower variances (Table 2.6).

2.4. Discussion

2.4.1. Ratio—A Dubious Matrix to Estimate NUE

Disparity in the functional relationship between AN and grain yield show that being a ratio, NUE could also be subjected to the same limitations of ratio analysis as previously demonstrated by Tanner (1949), Packard and Boardman (1988), Allison *et al.,* (1995), Raubenheimer (1995), Jasieński and Bazzaz (1999), and Beaupre (2005). This discrepancy in predicting the effect of AN on grain yield gives an important insight into the challenges that could be involved in accurately assessing NUE, which in turn can have interpretative and management implications.

Allison *et al.,* (1995) demonstrated that the ability of ratios to control for the effects of denominator on the numerator was dependent on a few statistical assumptions. Results from ratio analysis were only meaningful if the relationship between the two variables was isometric in nature i.e., the slope was constant and the line explaining the functional relationship was linear and passed through the point of origin (Packard and Boardman 1988; Raubenheimer 1995). Ratio analysis fails to account for a non-linear relationship between two variables, and fails to remove any confounding effect of the denominator, thus making ratio analysis a dubious matrix (Curran-Everett 2013). Our results showed that QR models performed better in comparison to the LR models, and yielded lower RMSE and $RMSE_n$. This observation confirmed that the relationship between grain yield and AN was non-constant, allometric in nature. These results were consistent with conclusions from earlier studies (Kaleem *et al.,* 2012; Poffenbarger *et al.,* 2017). According to these QR models, there were two phases of response curves; phase A and phase B. During phase A, AN improved the crop's ability to assimilate more N into the grain and hence, there was a positive grain yield response. However, per unit increase in grain yield decreased for every increment of AN until it became zero. The amount of AN where slope became zero marked the culmination of phase A. In phase B, grain yield reached its maximum and beyond this level of AN, NUE continued to decrease (McDonald and Hooper 2013). This curvilinear response disproved the assumption of linearity and constant slope, and showed that grain productivity was changing throughout the curve as some function of AN, as given by equation 2.8–2.10.

Results from the QR analysis were in accordance to response curves generated from field trials used to estimate agronomically optimum N rate (AONR) and economic optimum N rate

(EONR) (Rutan and Steinke 2017). These response curves can help farmers to identify maximum achievable yield which is represented by its summit. The corresponding value of N supply rate (fertilizer and AN) is known as agronomically optimum N rate (Sawyer *et al.,* 2006). Though, this represents the maximum yield that could be achieved, revenue drives these management decisions. Therefore, EONR is estimated from the response curve where the N supply rate generates enough revenue from gain in yield that it offsets the cost of its application (Heady *et al.,*1955; Sawyer *et al.,* 2006). This is indicated by the point on yield curve where slope is the same as the slope for LR model explaining the relationship between revenue and cost of N application. These yield response curves are used as a tool to help farmers make N fertilization management decisions.

In addition to the non-linear relationship between the two variables, NUE also deviated from the assumption of a zero intercept for the Lamoureux and Brad sites. Ratio analysis offers a reasonable means of controlling the effect of denominator on the numerator only when intercept is not significantly different from zero (Allison *et al.,* 1995; Curran-Everett 2013). However, for the Lamoureux and Brads site, this condition was not satisfied. Therefore, NUE as a ratio failed to provide a legitimate method to control for the effect of AN on grain yield for these sites. Failure to comply with this condition further illustrated the perils associated with defining NUE as a meaningful ratio. Defining NUE as per unit increase in grain yield to AN infers that the more soil N is available to the plants, the higher the grain yield. However, grain yield beyond a certain optimum of AN is limited by other agronomic and environmental factors, such as moisture and availability of other nutrients (Brancourt-Hulmel *et al.,* 1999; Raun and Johnson 1999; Fixen *et al.,* 2015). Therefore, one should be careful while drawing any conclusions using this definition of NUE, as N availability beyond the AONR can likely become detrimental to the grain productivity and quality, and the environment (Hong *et al.,* 2007).

2.4.2. Regression—An Alternative Heuristic Approach to Estimate NUE

Regression has been suggested as an alternate heuristic, as it alleviates some of the limitations of ratio analysis (Curran-Everett 2013). Regression analysis offers a flexible approach for hypothesis testing as it is not restricted by the necessity of a zero intercept of the regression of the variables of interest (Allison *et al.,* 1995). Before proceeding to LR, the assumption of normality should be satisfied. If the variables are not normally distributed, one needs to resort to non-parametric statistical tests for hypothesis testing. For all the sites, data for both variables exhibited a normal distribution. Comparing the results from ratio and LR model I analysis led to disparate conclusions. According to ratio analysis, the highest per unit increase in grain yield to AN was observed at Brad site; however, this per unit change was the lowest according to LR model I analysis. Contradicting results were also observed for Bert site where ratio analysis yielded the lowest per unit gain in grain yield contrary to the highest per unit gain according to LR model I analysis. These different conclusions are tethered to the problematic matrix of ratio analysis that obscures the true relationship between the variables of interest, hence leading to erroneous conclusions. To my knowledge, statistical challenges involved in accurate assessment of NUE in light of the limitations of ratio analysis have not been explicitly described before in scientific literature.

In addition to the theoretical flaws of a ratio, there are a few practical limitations to be considered as well, such as measurement errors associated with the explanatory variable (Curran-Everett 2013). The LR model I assumed there were no appreciable errors in the measurements of AN. However, soil test results are subjected to various sampling and measurement errors (Tan 2005), and these measurement errors are rarely taken into consideration. This failure can introduce bias in slope estimated through LR model I (Legendre and Legendre 2012). In such scenarios, it is recommended to use LR model II to predict this relationship among the two variables (Legendre 2000). In my study, results from LR model II were consistent with the findings of LR model I analysis, and led to the same conclusion where NUE was the highest at Bert site; whereas, it was the lowest at Brad site. Relatively smaller sample sizes used in this study might have concealed differences in NUE estimates from the two approaches. Therefore, it is recommended to use higher sample size for future studies. To my knowledge, the functional relationship between AN and grain yield has not been explicitly described before using LR model II.

The relationship between AN and grain yield was also modelled through the PWR model, where two interconnected LR lines fitted the data for different ranges of AN. The points of contact between these two fitted linear segments, known as the breakpoints, represented the value of AN beyond which slope of the linear function changed. These breakpoints offered valuable information of practical significance (Muggeo 2017) representing the amounts of AN beyond which the net per unit increments in grain yield noticeably decreased. This information can enable the farmers to make informed decisions as to whether fertilize their field given that the revenue grows faster than the cost of fertilizer application.

The QR model was the most robust model, as it illustrated the true dynamics of NUE, as given by the "law of diminishing returns" of plant growth proposed by Ehrlich Alfred Mitscherlich in 1909. This law stated that for every increment of fertilizer input, the growth response―in this case, grain yield response decreased (Mitscherlich 1909). The yield response reduced as a function of the first derivative for the given response curve. In contrast, the PWR model suggested that the relationship of AN and grain yield was explained by multiple linear segments, which in return, perpetuated constant per unit increase within the various ranges of AN. This observation made any simplified linear estimation of NUE a questionable approach to quantify the relationship between the two variables.

2.4.3. Sample Size—A Practical Limitation to Accurately Evaluate Genotypes Differing for NUE

Our results suggested that the evaluation of different wheat varieties for improved NUE required a large number of plots to observe a certain difference relative to control varieties (Table 2.6). To my knowledge, use of power analyses to estimate the minimum number of plots required to distinguish genotypes differing for NUE have not been reported before in the scientific literature. However, power analysis is an important preliminary step as it enables the plant breeders to design an experiment powerful enough to eliminate the probability of making type II error (Sullivan and Feinn 2012). These findings lead us to another statistical challenge that limits the accurate in-field assessment of NUE.

Given the large number of plots needed to evaluate the performance of NUE genotypes, financial and logistic limitations would make it difficult for the breeders to set up and manage trials with sufficient statistical power. Such intense requirements for infrastructure, labor, space, machinery and investment could hamper the practical application of this analysis.

2.5. Conclusion

This study provides evidence that statistical and practical limitations could hamper the accurate assessment of NUE. Defining NUE as a ratio of grain yield to any measure of N, in this instance, AN is a deceptively simple matrix that could lead to inaccurate conclusions. As shown in this study, the NUE as a ratio fails to meet the underlying assumption of isometry therefore, skewing the true relationship between the numerator and denominator. Among all the evaluated approaches, QR analysis is the best approach to estimate NUE, as it elucidates true quadratic relationship between grain yield and AN, and that is given by the first derivative of the quadratic equation.

In addition to statistical limitations, the challenges in implementing a trial with sufficient power to detect a substantive difference between the genotypes differing for NUE imposes a practical limitation. In many or perhaps most cases, a large sample size is required to achieve sufficient power for hypothesis testing. It is imperative to acknowledge these statistical and practical challenges while drawing any conclusion using ratio analysis as a mean to study NUE.

2.6. Figures and Tables

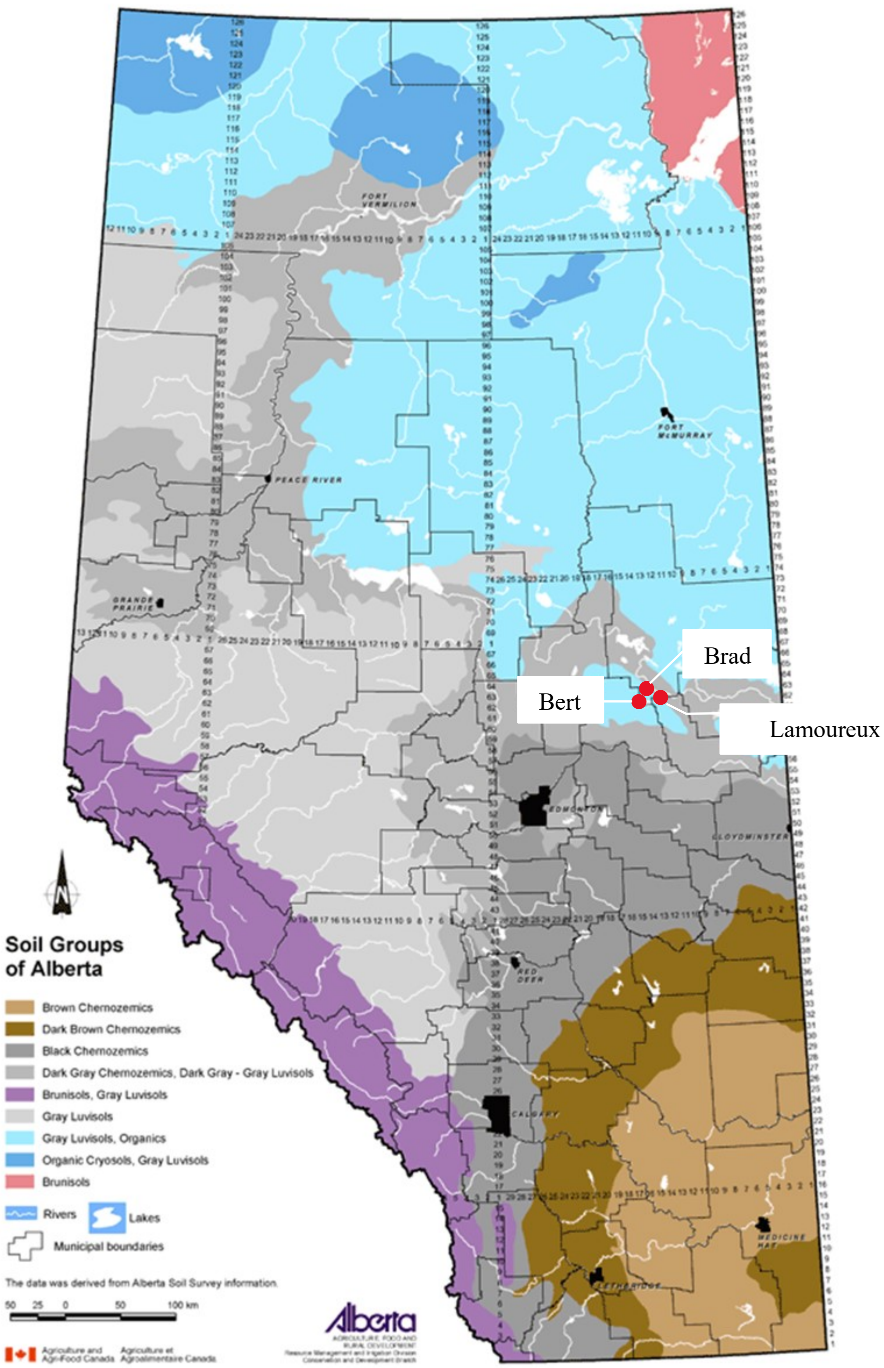


Figure 2.1. Map showing soil groups of Alberta. The geographic location of three study sites is indicated by red dots. Image courtesy: Alberta Agriculture and Forestry.

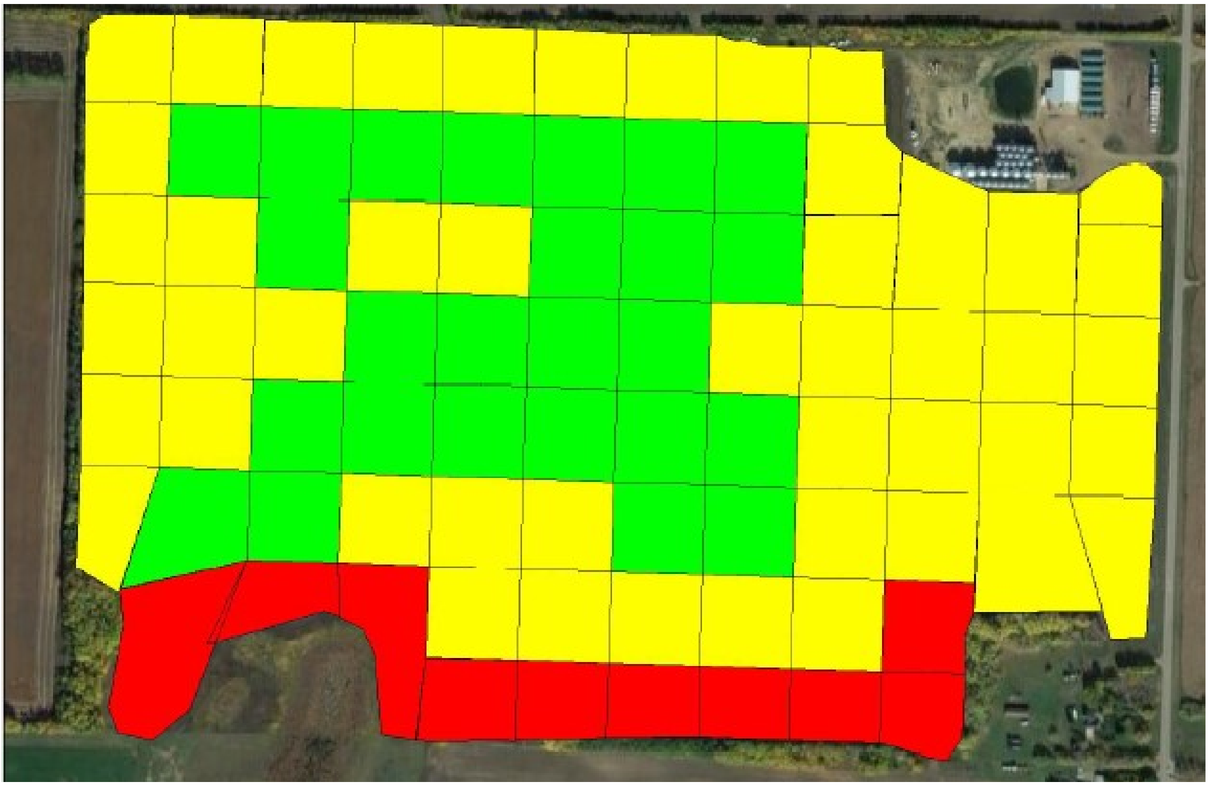


Figure 2.2 (a). Variable rate application of urea (46-0-0) to the Bert site for year 2015. Green, yellow and red pixels illustrate 120, 100, and 87 lbs ac^{-1} of applied urea.

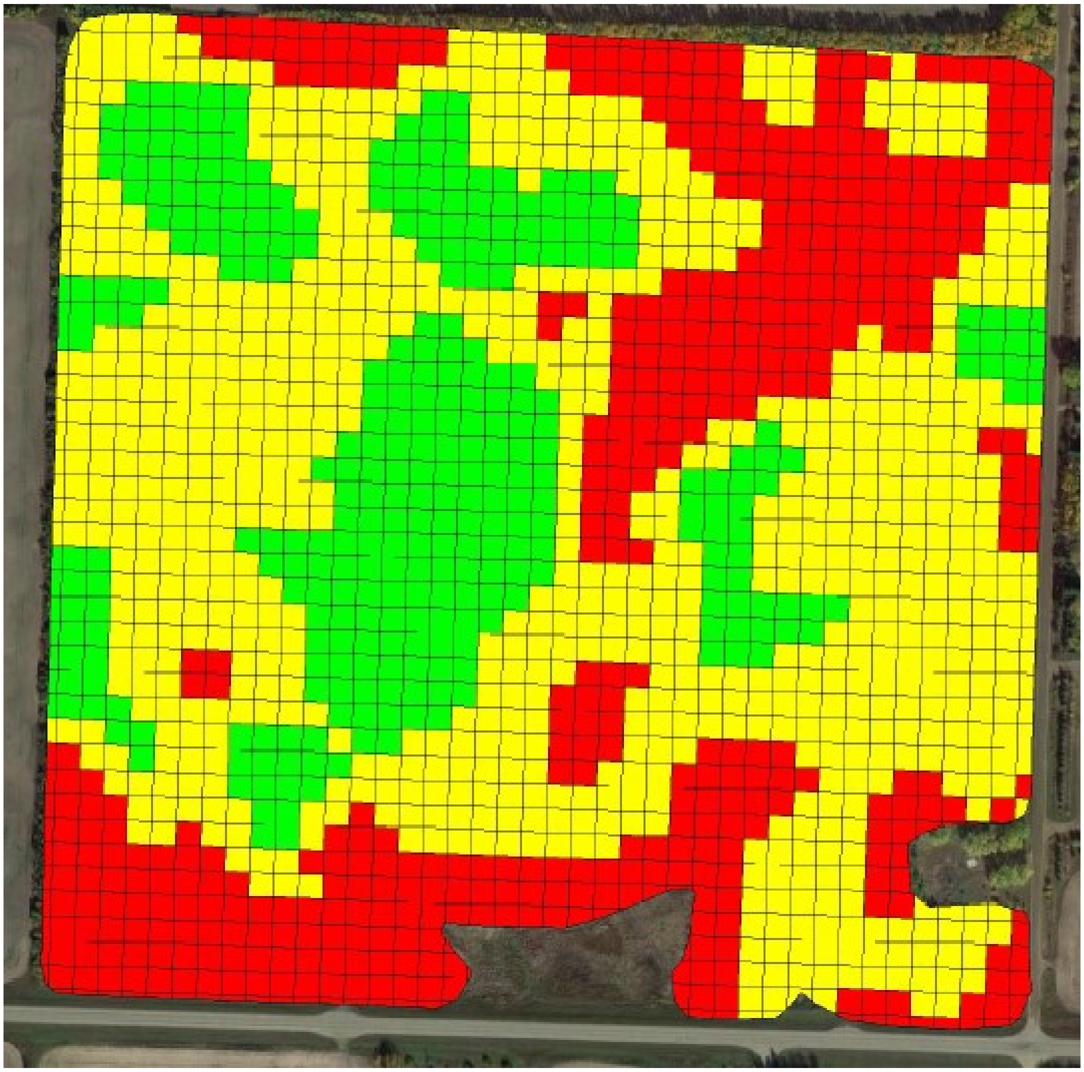
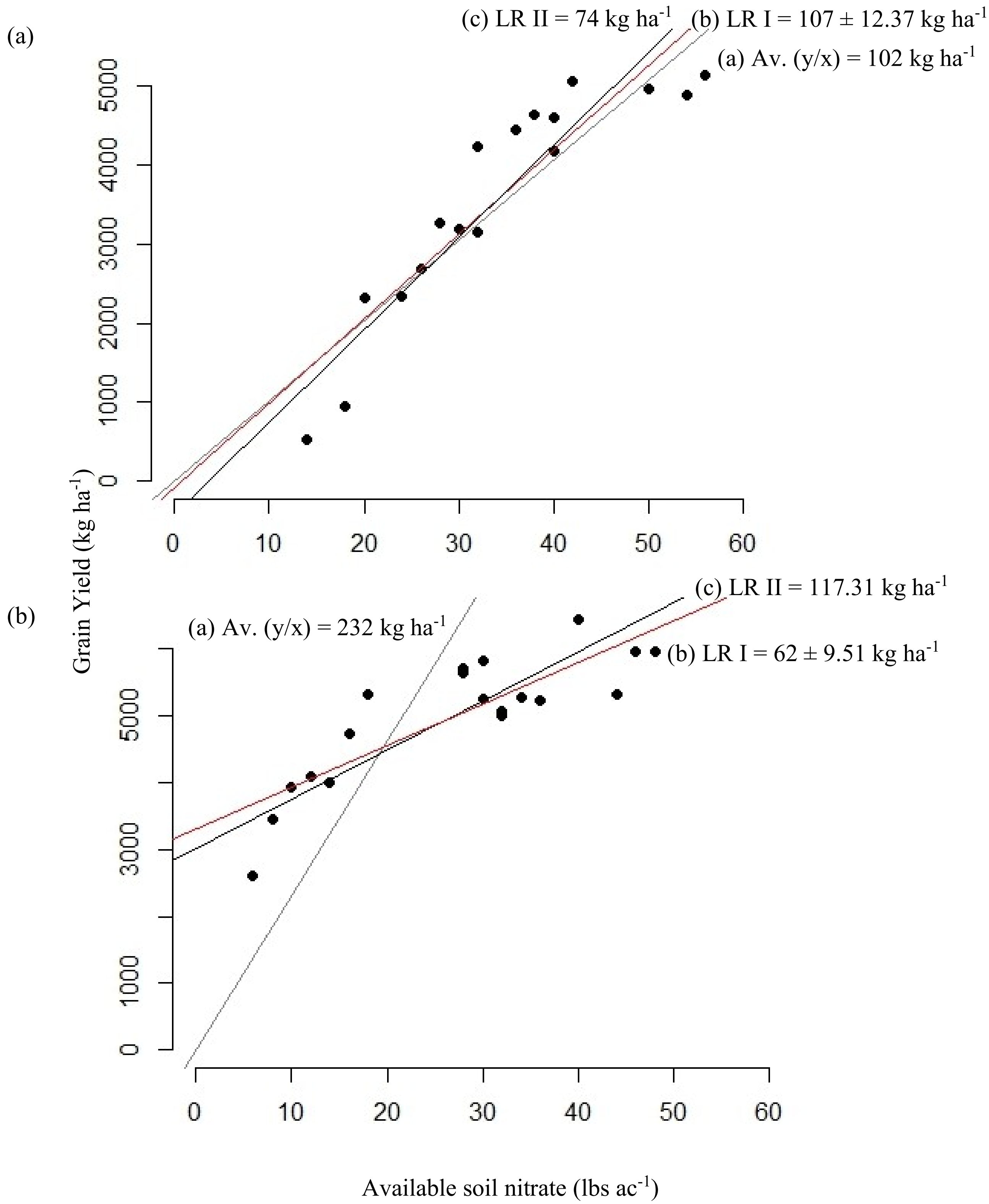


Figure 2.2 (b). Variable rate application of urea (46-0-0) to the Lamoureux site for year 2015. Green, yellow and red pixels illustrate 76, 65, and 54 lbs ac^{-1} of applied urea.

Figure 2.2 (c). Variable rate application of urea (46-0-0) to the Brad site for year 2015. Green, and red pixels illustrate 130, and 110 lbs ac^{-1} of applied urea.



(a)
(c) LR II = 74 kg ha-1
(b) LR I = 107 ± 12.37 kg ha-1
(a) Av. (y/x) = 102 kg ha-1
(b)
(a) Av. (y/x) = 232 kg ha-1
(c) LR II = 117.31 kg ha-1
(b) LR I = 62 ± 9.51 kg ha-1
Grain Yield (kg ha-1)
Available soil nitrate (lbs ac-1)

(c)

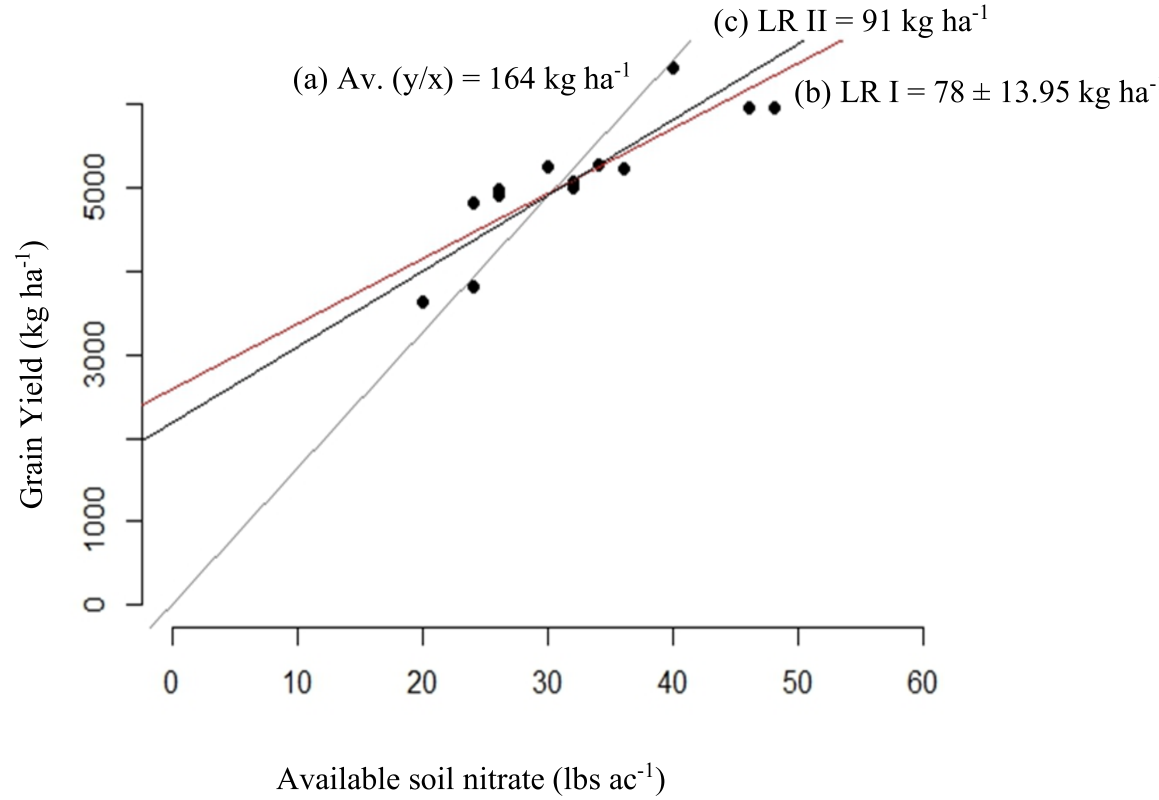
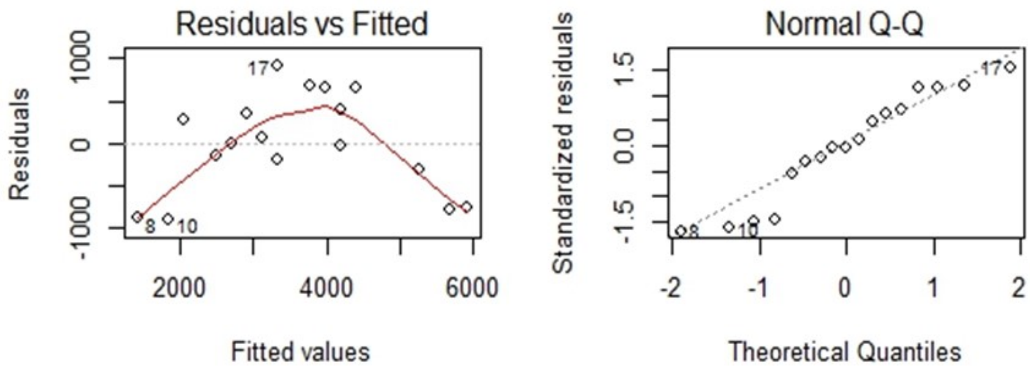
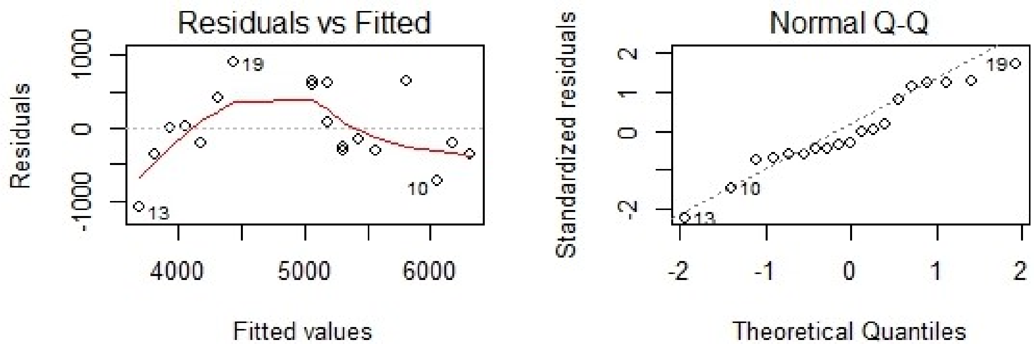


Figure 2.3. Exploration of the relationship between available soil nitrate (AN) and wheat grain yield for the Bert (a), Brad (b), and Lamoureux (c) sites. Line A (shown in gray) shows on an average, there was an increase of 102, 232, 164 kg ha^{-1} in grain yield for every lb ac^{-1} of AN at the Bert, Brad, and Lamoureux sites, respectively. Line B (shown in red) and C (shown in black) show that the estimates of slope using linear regression model I and linear regression model II were 107 ± 12.37 kg ha^{-1} and 117 kg ha^{-1} for Bert, 62 ± 9.51 kg ha^{-1} and 74 kg ha^{-1} for Brad, and 78 ± 13.95 kg ha^{-1} and 91 kg ha^{-1} for Lamoureux site, respectively.

(a)



(b)



(c)

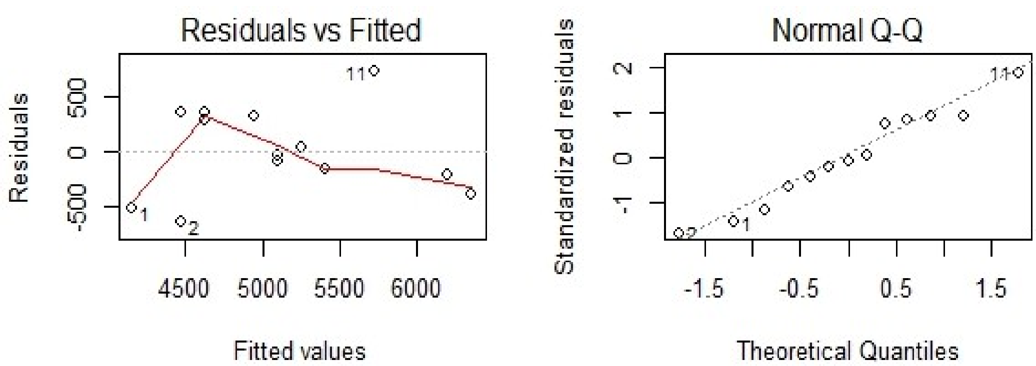


Figure 2.4. Regression diagnostic plots showing fit of the linear models for the Bert (a), Brad (b), and Lamoureux (c) sites. Plots of residuals versus fitted values in the left panels showed patterns in dispersion of points around a horizontal line, which should otherwise be a roughly straight line in order to meet the assumption of linearity of the residuals. This indicates that these linear models

do not perform well in terms of modelling the data for these sites. Q-Q plots in the right panels show residuals aligning closely to the diagonal lines indicating that residuals are normally distributed.

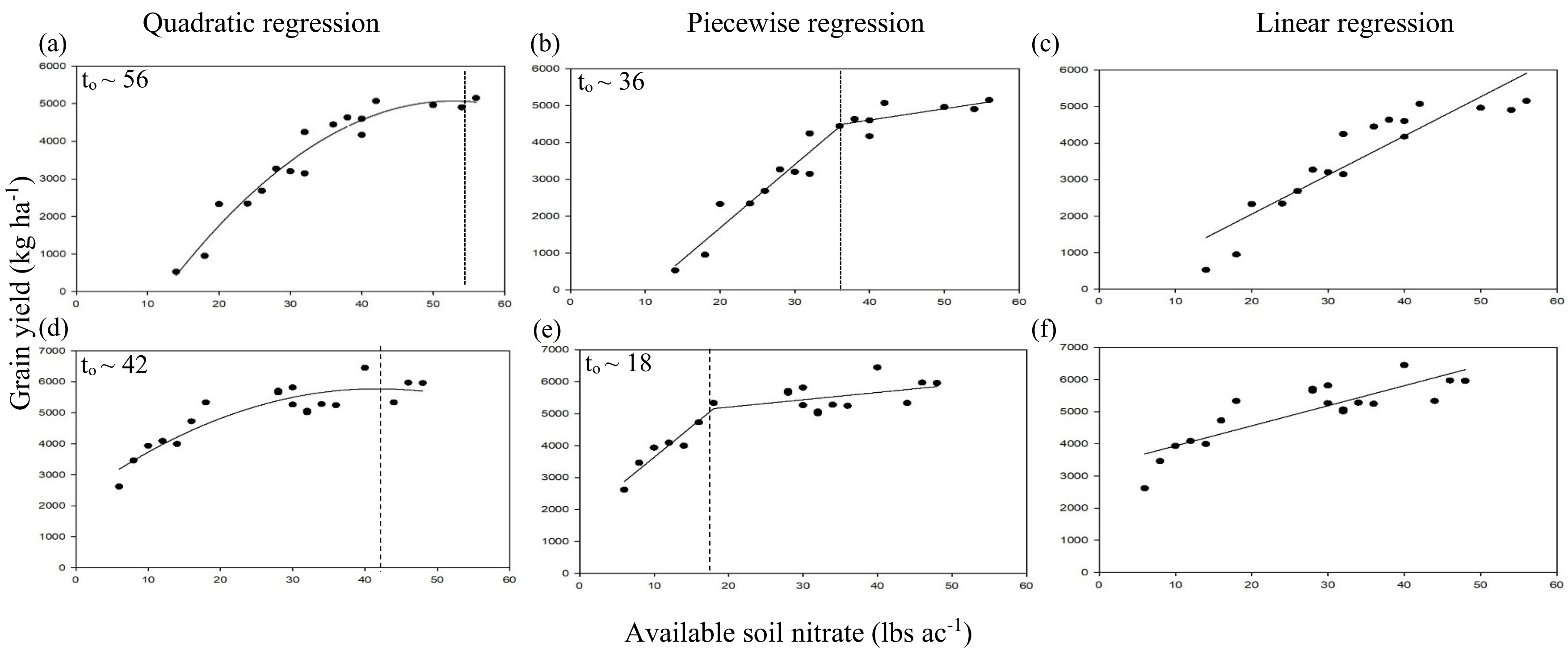


Figure 2.5. Regression analysis of nitrogen use efficiency (NUE) in wheat. NUE for each of our three study sites; Bert (a-c), Brad (d-f), and Lamoureux (g-i) was modelled using grain yield and available soil nitrate (AN) data. Grain yield was monitored in Fall 2015 using Green Star Monitor 3 mounted combine harvester. Spring soil samples were collected during June of the same year from a 2-ha grid at a depth of 0-15 cm using AutoProbe™ from each site. Soil samples were sent to Midwest lab for soil fertility analysis. These acquired data sets were modelled using linear, quadratic regression (QR) and piecewise regression (PWR) analysis in R software. Dotted vertical lines show the threshold (t_o) for respective model, beyond which yield response either became zero (as in case of QR model), or reduced (as shown by PWR model).

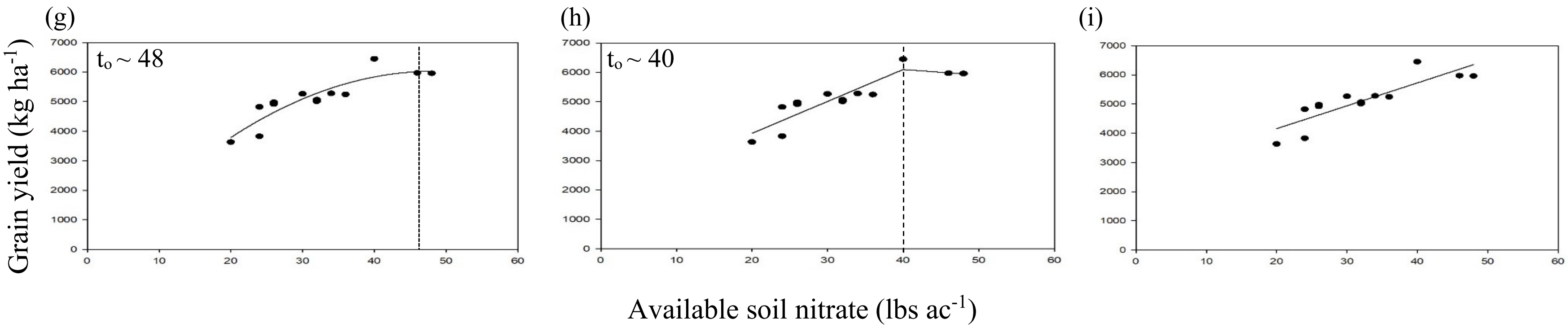


Figure 2.5. (continued)

Table 2.1. Soil N (applied N fertilizer and available soil N) and measured wheat yield at the Bert site in 2015. Peas was grown at this site in 2014.

Applied N fertilizer (lbs ac^{-1})	**Measured AN (lbs ac^{-1})**	**Measured Yield (kg ha^{-1})**
120	26	2683.3
87	42	5070.7
120	20	2326.9
87	40	4599.9
100	38	4633.6
87	50	4963.1
100	32	3147.3
120	14	524.6
100	30	3201.1
120	18	948.2
87	54	4902.6
100	36	4445.3
120	24	2340.3
100	40	4169.6
87	56	5151.4
120	28	3268.4
100	32	4243.5

Table 2.2. Soil N (applied N fertilizer and available soil N) and measured wheat yield at the Lamoureux site in 2015. Canola was grown in 2014 at this site.

Applied N fertilizer (lbs ac^{-1})	**Measured AN (lbs ac^{-1})**	**Measured Yield (kg ha^{-1})**
76	20	3631.56
76	24	3826.59
76	24	4821.9
65	26	4976.58
76	26	4916.05
76	30	5265.76
65	32	5064.01
76	32	5010.2
65	34	5279.21
65	36	5245.58
65	40	6449.38
54	46	5971.89
54	48	5958.44

Table 2.3. Soil N (applied N fertilizer and available soil N) and measured wheat yield at the Brad site in 2015. Canola was grown in 2014 at this site.

Applied N fertilizer (lbs ac^{-1})	Measured AN (lbs ac^{-1})	Measured Yield (kg ha^{-1})
130	28	5709.62
130	28	5655.81
130	30	5265.76
130	30	5817.22
100	32	5064.01
130	32	5010.2
110	34	5279.21
110	36	5245.58
110	40	6449.38
110	44	5333.01
110	46	5971.89
110	48	5958.44
130	6	2616.07
130	8	3463.43
130	10	3934.19
130	12	4088.87
130	14	3994.71
130	16	4727.75
130	18	5333.01

Table 2.4. Descriptive statistics for data variables.

Site	Data variables	Mean	St.dev.	CV (%)	Skewness	Kurtosis
Bert	NUE	102	24.53	24	-1.28	0.96
(n = 17)	Grain yield (kg ha^{-1})	3566	1428.24	40	-0.70	-0.74
	AN (lbs ac^{-1})	34	12.17	36	0.20	-1.01
Brad	NUE	232	105.68	45	0.74	-0.97
(n = 19)	Grain yield (kg ha^{-1})	4996	974.53	19	-0.78	-0.22
	AN (lbs ac^{-1})	27	13.22	49	-0.08	-1.35
Lamoureux	NUE	164	23.31	14	-0.08	-1.17
(n = 13)	Grain yield (kg ha^{-1})	5109	780.56	15	-0.27	-0.56
	AN (lbs ac^{-1})	32	8.58	27	0.46	-1.05

NUE: nitrogen use efficiency; AN: Available soil nitrate (lbs ac^{-1})

Table 2.5. Regression parameters for quadratic, piecewise and simple linear regression models.

Site	Models	RMSE (kg ha^{-1})	$RMSE_n$ (%)
Bert	Quadratic	347	2.14
	Piecewise	357	2.13
	Linear	602	3.83
Brad	Quadratic	437	1.83
	Piecewise	379	1.54
	Linear	534	2.31
Lamoureux	Quadratic	376	1.79
	Piecewise	384	1.73
	Linear	415	2.07

RMSE: root mean square error (kg ha^{-1}); $RMSE_n$: normalized root mean square error (%).

Table 2.6. Estimated number of samples needed to detect a difference of 10% in nitrogen use efficiency relative to the mean of the check variety, AC Andrew, at a significance level of 95% (α = 0.05) and power of 80% (β = 0.8).

Variety	Mean NUE	NUE Variance	Minimum Sample Size (plots per hybrid/ line)
Plentiful	232	11,168.26	969
Harvest	164	543.35	47
AC Foremost	102	601.72	53

NUE: nitrogen use efficiency

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Chapter 3: Comparative Assessment of Soil Fertility Parameters Using Non-Geostatistical and Geostatistical Approaches

3.1. Introduction

Spatial heterogeneity in soil properties across the landscape can be conceptualized as a function of interactions between intrinsic (e.g., topography, soil, and vegetation type) and extrinsic (e.g., management practices and climate) factors (Cambardella *et al.,* 1994; Diacono *et al.,* 2013; Qiu *et al.,* 2016). At first, the resulting spatial variability appears to be random due to complex and dynamic interactions between these factors. Significant variability in physical and chemical soil properties exists across a landscape, and this variability poses a challenge in farm management from both economic and environmental standpoint (Komatsuzaki and Ohta 2007). By explicitly unveiling and documenting spatial patterns, precision mapping offers a solution to this problem, and enables managers to make informed management decisions (Diacono *et al.,* 2013). However, success of this technology hinges on the accurate assessment and quantification of the underlying soil variability.

The development of sophisticated global positioning systems (GPS) and powerful software have recently prompted the integration of geostatistics into agricultural and environmental management. Geostatistics relies on spatial autocorrelation to generate a continuous surface from point data, and interpolates the given variable at unsampled locations with an estimate of reliability (Oliver and Webster 2014; Li and Heap 2014). Since the advent of this field, a number of different interpolation methods have been developed—some more robust than the others.

Kriging is a geostatistical equivalent of least square regression that yields best linear unbiased predictions at any unsampled location (Noel 1990). Univariate kriging methods, such as ordinary kriging (OK) have been used to predict soil fertility profiles across different landscapes

(Xing-Yi *et al.,* 2007; Mueller *et al.,* 2010; Vasu *et al.,* 2017). However, OK may have inadequate predictive power to develop accurate predictive maps (Li and Heap 2011). In such scenarios, sample size may limit the reliability of the derived inference, as the estimate of spatial autocorrelation, may be erroneous (Oliver and Webster 2014).

Recently, combined interpolation methods, such as regression kriging (RK), have been employed to predict and subsequently map different soil properties. RK is stochastic extension of regression analysis that involves kriging of the residuals obtained from regressing the response variable as a function of auxiliary variables (Hengl *et al.,* 2004). Different case studies have shown that RK performs better as compared to other competitors including inverse distance weighting interpolation, OK, and ordinary cokriging (OCK) (Hengl *et al.,* 2007; Meng *et al.,* 2013). However, lack of a user-friendly geoprocessing environment limits widespread adoption of RK. Furthermore, regression analysis becomes increasingly difficult if plethora of auxiliary variables are available.

Theoretical and practical aspects of these spatial interpolation methods (SIMs) have continued to evolve, and this has led into the development of multivariate kriging methods, such as OCK. OCK is becoming increasingly popular due to easy access to high resolution remote sensed data, such as Light Detection and Ranging (LIDAR), and improved computational power. Among other pedogenic factors, topography has been widely used to model different pedogeomorphological processes, including soil fertility (Song *et al.,* 2014), and soil hydrology. Although many studies have documented improvement in quantification of underlying spatial heterogeneity using OCK (Bogunovic *et al.,* 2017; Guenette and Hernandez-Ramirez 2018), some studies have also shown that use of OCK may deteriorate the predictive accuracy when compared to its univariate and hybrid counterparts, such as OK and RK, respectively (Peng *et al.,* 2013; Bogunovic *et al.,* 2017).

Topography is one of the most important attributes of agronomic fields that affects the paradigm of spatial distribution of soil through erosion and deposition (Moulin *et al.,* 1994). Thus, spatial distribution of various intrinsic pedogenic processes, including soil fertility and soil hydrology, are also affected by topography due to redistribution of soil particles (Bakhsh *et al.,* 2000). Crop productivity is the product of interactions between these edaphic variables. Moreover, environmental factors also exert significant effect on crop productivity. The easy availability of remote sensing data offers new realms for quantifying and managing variability in crop productivity. Studies have been conducted to decipher the relationship between crop productivity and topographic variables, such as slope, elevation, curvature and aspect (Moulin *et al.,* 1994; Iqbal *et al.,* 2005; Kumhálová *et al.,* 2011; Heil *et al.,* 2018). However, the relationship between topography and crop productivity is poorly understood, and there is a paucity of studies within the Canadian Prairies

Several studies have been conducted to quantify the spatial dependency of soil fertility in agricultural fields; however, there is a knowledge gap in the relative performance of typical spatial interpolation methods, particularly in Canadian Prairies. To achieve the ultimate goal of tailoring inputs to spatially-varying crop requirements, it is imperative to develop accurate soil maps. Therefore, research objectives for this project were: (i) to quantify the spatial variability in soil fertility profile at a field scale, (ii) to compare performance of regression and geostatistical models with an aim to identify an optimal spatial model, (iii) to determine if multivariate kriging outperforms univariate and hybrid kriging methods by the addition of LIDAR derived terrain covariates, (iv) to estimate minimum number of sample size needed to predict each variable with a certain degree of precision, and (v) to decipher relationship between crop productivity and topographic attributes, such as aspect, slope, elevation, curvature, and hillshade.

3.2. Materials and Methods

3.2.1. Study Sites

This study was conducted at two commercial sites privately owned and managed by Kalco Farms Ltd. These study sites were located north of Edmonton in Sturgeon county. The Lamoureux site (53°50'06.5"N, 113°12'14.5"W) had a total area of approximately 60 hectares (ha) with a wheat (*Triticum aestivum* L.)–canola (*Brassica napus* L.) rotation. The Bert site (53°51'13.4"N, 113°14'06.8"W) employed wheat–canola–field pea (*Pisum sativum* L.) rotation on an area of 78 ha. Farm operations included light tillage in early May for even distribution of crop residue and weed control. Soil type at both sites was characterized as Black Chernozem according to Canadian System of Soil Classification. Based on data collected over 15 years from the nearest weather station, approximately 15 km away from these sites, climate was characterized by mean annual precipitation and air temperature of 730 mm and 2.67 °C, respectively.

3.2.2. Soil Data Collection

During June 2014, the Bert study site was sampled at 82 locations with 95 m between each sampling point on a 1 ha (2.5 acre) grid using a tractor driver AutoProbe ™ soil sampler. A total of 20 samples were collected from each grid at a depth of 0-15 cm followed by homogenization to get one representative sample per grid. The centre of each grid was geo-referenced as a sampling location for that grid. The collected samples were added to pre-labelled sampling bags, and were stored at 4°C prior to shipping to Midwest laboratories for soil fertility analysis.

An area of 8 ha was sampled at 36 georeferenced locations at the Lamoureux site during June 2017 at a distance of 56 m, and an additional 20 samples were collected from two transects at a distance of 4 m. Sampling equipment and handling was the same as that for Bert site, except for the sampling intensity and distance.

3.2.3. Derivation of Terrain Covariates from LIDAR Data

Topographic LIDAR data was acquired via Cessna aircraft equipped with Leica sensors with cloud datapoints integrated to a resolution of 2 m x 2 m with a corresponding horizontal and vertical accuracies of 50 and 30 cm, respectively. A suite of terrain covariates including elevation, aspect, hillshade, slope, and curvature were used to describe land surfaces. Candidate terrain covariates were derived using Spatial Analyst Tools from ArcGIS ver. 10.5.1 (ESRI, Redlands, CA, USA). After extracting area of interest for both sites, rasters for aspect, hillshade, slope and curvature were developed using the "surface" tool. Elevation data were extracted for each 2 m x 2 m grid cell followed by "sampling" all the developed rasters using bilinear interpolation into a .dbf file.

3.2.4. Statistics

Sample statistics including mean, standard deviation, minimum and maximum values, and coefficient of variation (CV) (Table 3.1) were calculated to describe different soil fertility parameters of our study sites. Exploratory data analysis, such as visual analysis of Q-Q plots was conducted to explore datasets for the presence of outliers. Prior to multiple linear regression (MLR) analysis, the assumption of normality was tested using the Kolmogorov-Smirnov (KS) test. Measures of kurtosis and skewness (Table 3.1) were used in conjunction with KS test to identify non-normal variables, and were log transformed where deemed necessary. Auxiliary variables were pre-screened based on strength and level of significance of their functional relationship with the response variables (Table 3.2). Variables with high variance inflation factor (VIFs > 4) were eliminated from the respective maximal models to avoid multicollinearity among auxiliary variables. The model with the lowest Akaike's Information Criterion (AIC) was selected as the optimal model (Table 3.3), and were tested for assumption of normality and homoscedasticity of residuals through the KS test and visual examination. Residuals obtained from MLR analysis were subsequently used in RK for spatial structural analysis and interpolation. The data analysis was completed using R ver. 3.3.3 (R Foundation for Statistical Computing, 2017). The relationship between grain productivity and terrain attributes was explored using Pearson correlation analysis in SigmaPlot ver. 11.1. (SYSTAT 2008) (Table 3.4).

3.2.5. Geostatistics

The spatial structure of each soil fertility parameter was deciphered using a combination of different standard, including OK and OCK, and combined geostatistical methods, such as RK. Estimation of the semivariogram constituted the preliminary step for each one of these geostatistical analysis methods, and was used to quantify variation in soil fertility parameters as a function of distance. The developed semi-variogram was a graphical representation of the magnitude of this spatial auto-correlation, where spatial auto-correlation statistic—semivariance, was plotted against distance. Semivariance for a given sampling interval can be calculated using the following formula:

$$\gamma(h) = \frac{1}{2(N)} \sum_{i=1}^{N} (Zi - Zi + h)^2 \qquad [3.1]$$

where; γ(h) is the semivariance for sampling pairs separated by distance h, Z_i and Z_{i+h} are the measured sample values at locations separated by distance h.

This iterative modelling exercise was completed in ArcGIS ver. 10.5.1 (ESRI, Redlands, CA, USA). Active lag distance, which defined the distance over which spatial autocorrelation statistic was calculated, covered 50-75% of the maximum sampling distance. A minimum of 30 pairs were used to populate each lag class, and lag class distance intervals were selected accordingly. After calculating semivariance for each class, a spherical, exponential, gaussian or linear model was fitted (Figure 3.1 & 3.2, Table 3.5). After modelling the spatial dependence of each soil fertility parameter using semivariogram, the underlying spatial structure was interpolated using three types of kriging. The general estimation formula for OK, OCK and RK are presented in the following equations:

$$OK = \hat{Z}_i = \sum_{i=1}^{N} \lambda_i Z_i \quad [3.2]$$

$$OCK = \hat{Z}_i = \sum_{i=1}^{N} a_i Z_i + \sum_{i=1}^{N} b_i Z_j \quad [3.3]$$

$$RK = \hat{Z}_i = Z_i(R) + \sum_{i=1}^{N} \lambda_i\, e(Z_i) \quad [3.4]$$

where; $\hat{Z}_i$ and Z_i are the predicted value and measured value for the variable of interest at location i, Z_j is the measured value for the covariate, N is number of samples, λ_i, a_i, and b_i are the kriging weights assigned to the measured value, $Z_i(R)$ is the estimated value of variable Z_i by the regression model, and $\lambda_i\, e(Z_i)$ is the residual for the given location i.

A series of additional steps were completed for OCK due to inclusion of covariates. Similar to primary variables, in this case—soil fertility parameters, spatial autocorrelation for each covariate was also explored through semivariogram. Cross-correlation between primary and secondary variables was given by cross-variogram, and it established cross-continuity between the two variables as a function distance, and cross-correlation was calculated using following formula:

$$Z_{ij} = Z_{ji} = \frac{1}{2N\ (h)} \sum_{i\ =\ 1}^{N(h)} [Z_{\ (i+h)} - Z_i]\ x\, [Z_{j(j+h)} - Z_j] \qquad [3.5]$$

where; Z_{ij} and Z_{ji} is the cross-correlation between variable i and j, N is number of samples, h is the distance between two sampling points, Z_i and Z_{i+h} are the measured sample values of the primary variable at locations separated by distance h, Z_j and Z_{j+h} are the measured sample values of covariate at locations separated by distance h.

3.2.6. Cross-validation

Cross-validation is a leave-one-out method that removes one measured value at a time, and uses the developed model to re-estimate the removed value from the remaining values of the dataset. It is performed to test accuracy of the developed predictive models. Different diagnostic accuracy statistics, including root mean square error (RMSE), mean square error (MSE), and mean absolute error (MAE) are used for this purpose, and these are defined in the equations below:

$$MSE = \frac{1}{n} \sum_{i\ =\ 1}^{n} (Z_i - \hat{Z}_i)^2 \qquad [3.6]$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i\ =\ 1}^{n} (Z_i\ -\ \hat{Z}_i)^2} \qquad [3.7]$$

$$MAE = \frac{1}{n} \sum_{i\ =\ 1}^{n} (Z_i - \hat{Z}_i) \qquad [3.8]$$

where; $\hat{Z}_i$ and Z_i are the predicted value and measured value for the variable of interest i, *and* n is number of samples.

3.2.7. Estimation of Minimum Sample Size

Minimum sample size was calculated to estimate the number of soil samples required to predict each soil fertility parameter with the desired level of accuracy (Table 3.7). For this study, accuracy levels of 10%, 20% and 50%, and probability of type I errors i.e., alpha (α) was set to 0.05 and 0.1. This set criteria provided reasonable spread of accuracy thresholds and statistical significance levels that were flexible enough to accommodate the accuracy needs of the upcoming studies. Sample sizes were calculated using the following equation given by Metcalfe et al. (2008);

$$N = \left(\frac{t_{\alpha}\, CV_{sill}}{D}\right)^2 \qquad [3.9]$$

where; N is the number of samples, t_{α} is the t statistic for the given alpha value ($t_{0.05} = 1.96$, $t_{0.1} = 1.645$), CV_{sill} is the measure of spatial variability within data for a given variable and is calculated using, $CV_{sill} = \frac{\sqrt{2 \text{ x } (C_o + C)}}{\bar{X}}$ (where; $C_o + C$ is the semivariogram sill, and $\bar{X}$ is the sample mean), and D is the required accuracy level.

3.3. Results and Discussion

3.3.1. Descriptive Statistics

Descriptive statistics for soil fertility parameters outlined important characteristics of each property at our study sites (Table 3.1). Visual inspection of the Q-Q plots identified three outliers in our data set from the Bert site. These were removed from the subsequent analysis. Data for some of the variables failed to comply with the assumption of normality, and were log transformed (base 10). Coefficient of variation (CV), in particular, gave an invaluable insight into the heterogeneous extent of our variables of interest. As described by Wilding (1985), CV was used to characterize each variable as weakly (CV < 15%), moderately (CV 15-35%), and highly (CV > 35%) variable (Table 3.1). In general, available soil nutrients were highly variable, as given by large indices of C.V. at both sites. These estimates of variability were consistent with studies conducted by Gallardo and Paramá (2007), Fu *et al.* (2010), Wang *et al.* (2009), and Vasu *et al.* (2017). Moreover, moderate variability was observed for cation exchange capacity (CEC) and organic matter (OM) at both study sites. This observation was in agreement with the findings of Cassel *et al.* (2010), Ferreiro *et al.* (2016), and Emamgholizadeh *et al.* (2017). Moderate to high estimates of variability for each of these soil fertility parameters could be explained through dynamic interactions of intrinsic and extrinsic factors functioning on different scales, thereby imparting spatial variability across the landscape (Lofton *et al.,* 2010). Available soil nitrate (AN), in particular, had high variability due to its strong propensity to move through the soil given its high water solubility and low affinity for soil surfaces, typically dominated by negative charges.

3.3.2. Step-wise Multiple Linear Regression Analysis of Soil Fertility Parameters

Selection of predictors is important to yield meaningful results. Therefore, it is crucial to make knowledge-based decisions and only to include biologically plausible candidate predictors. It is also imperative to draw a distinction between causation and association. Statistically, modelling a response variable as a function of association with another variable precludes from developing meaningful results, and may result in spurious conclusions. Prior to MLR analysis, variables were classified as response or/ and predictor (Table 3.1) based on our objective of model evaluation, and rationale of biological processes. Step-wise MLR analysis was conducted in order to generate baseline information for model evaluation. Akaike's Information Criterion (AIC) values served as a criterion for optimal model selection, as it measured how parsimonious the models were (i.e., the ability to predict the most variability with the least amount of predictors). Models with the lowest AIC values were selected as optimal models. The predictive capabilities of these models were better for soil fertility parameters exhibiting weak to moderate variations; for instance, CEC, OM and pH, with an R^2 generally higher than 0.5, but were unable to sufficiently predict highly variable soil nutrients at both sites (Table 3.3).

3.3.3. Semi-variography for Primary and Secondary Variables

Kriging-based SIMs rely on semi-variogram to generate weighted estimates of spatial autocorrelation at a given distance, and the developed algorithm is used to make predictions at unsampled locations (Oliver and Webster 2014). Isotropic semi-variograms were developed for each primary and secondary variable. The possibility of directional influences was also investigated through development of anisotropic semi-variograms and these influences were deemed insignificant if ratio of major to minor axis was less than 2.5. However, direction-dependent spatial autocorrelations were not detected. This might be due to insignificant influence of topography and other intrinsic soil processes, such as soil water movement, on inherent soil variability (Noorbakhsh *et al.,* 2008).

Understanding spatial dependence of each variable of interest is instrumental in deciphering, and subsequently mapping the underlying spatial structure (Webster and Oliver 2000). Estimation of different parameters of semi-variogram helped to quantify the spatial dependence for each variable. Cambardella *et al.* (1994) proposed a system of classification to quantify the extent of spatial continuity through analysis of nugget to sill ratio (NSR), where each variable is classified as weakly (NSR > 0.75), moderately (NSR = 0.25-0.75) or strongly (NSR < 0.25) dependent over space. Nature and extent of the prevalent soil variability can be attributed to intrinsic or extrinsic factors (Cambardella *et al.,* 1994). Intrinsic factors constitute inherent soil variability, and may be responsible for imparting strong spatial structure, and therefore, less variability. Whereas, extrinsic factors, such as different farm management practices, would result in weak spatial dependence. Analysis of NSR showed strong spatial dependence for all the soil properties at both sites, as substantiated by NSR values smaller than 0.25. There was however an exception to this observation as AN was weakly variable and CEC was moderately variable at the Bert site (Table 3.5). pH was also moderately variable at Lamoureux site (Table 3.5). Strong spatial dependencies for the studied soil fertility parameters were congruent with the findings of Cambardella *et. al* (1994), Omonode and Vyn (2006), Cemek and Mustafa (2007) and Guenette and Hernandez-Ramirez (2018), and were suggestive of low variability for a given variable of interest at a scale smaller than minimum sampling distance. These could be attributed to an intrinsic component of soil variability. Moderate variability of a soil property, in this instance, AN could be attributed to the cumulative effect of both inherent soil variability and management practices (Cambardella *et al.,* 1994).

3.3.4. Performance Assessment of Evaluated Statistical and Geostatistical Methods

Different geostatistical SIMs including OK, OCK, and RK were evaluated to study spatial variability of different soil fertility parameters at two study sites near Edmonton. Prediction error statistics, including RMSE, MSE, and MAE were primary means for assessing model performance (Table 3.6). The adequacy of R^2 as a matrix for model performance evaluation is questionable despite being commonly reported as a measure of goodness of fit, and therefore, was not used for model selection. The best performing method was characterized by smaller values of error statistics. Geostatistical SIMs performed better in estimating soil nutrient concentrations at both sites. However, the predictive performance of these methods was inconsistent for pH, CEC, and OM with MLR models outperforming geostatistical models at the Bert site (Table 3.3). Despite the best performance, estimates from MLR analysis were subjected to practical limitations because strong spatial structure (as illustrated by the semi-variogram analysis) rendered the residuals spatially auto-correlated. This violated the assumption of independent errors for MLR (Wagner 2013).

Of all the evaluated geostatistical and non-geostatistical methods, OK generally proved to be the most effective method to estimate soil nutrients at both sites, as illustrated by lower cross-validation error statistics. Highest performance estimates of OK for AN, AK (readily available potassium) and AP (readily available phosphorus; with exception to AN and AP at the Bert site) were inconsistent with the findings of Bogunovic *et al.* (2017) and Guenette and Hernandez-Ramirez (2018), where they concluded OCK was the front runner SIM. This disparity in conclusions could be explained in part by the poor correlation between soil nutrient profile and terrain covariates (Table 3.2). Strong correlation between primary and secondary variable is an important prerequisite that warrants reduction in error variance as suggested by Ahmed and De Marsily (1987), Hernandez-Stefanoni and Ponce-Hernandez (2006), Li and Heap (2011), and Meng *et al.* (2013). OCK was optimal SIM for predicting AP at Bert. This result supported work conducted by Bogunovic *et al.,* (2017). Improvement in performance of OCK, even in absence of correlation between the primary and secondary variable as in our case with elevation, may be partially explained by Borůvka *et. al.,* (2002), who pointed-out the limitations of conventional correlations to detect spatial correlations between variables. RK reduced error estimates in predicted AN at the Bert site, and these results complied with findings of Peng *et al.,* (2013).

Regression kriging was also the best performing SIM for estimates of pH at both sites, with smaller RMSE, MSE and MAE. This observation; however, was contrary to findings of Bogunovic *et al.* (2017), and Guenette and Hernandez-Ramirez (2018). According to their studies, OK and OCK were optimal SIMs to map pH at a farm scale. Additionally, RK predictions for OM and CEC at both sites were most reliable in our study. In multiple studies conducted by Bogunovic *et al.* (2017) and Bogunovic *et al.* (2017), OK and OCK were the most accurate SIMs for predicting OM. To the best of my knowledge, comparison-based studies focusing on performance assessment of different SIMs for predicting CEC are not available in the scientific literature. Superior performance of RK in comparison to other evaluated models may be due to strong correlation between response and predictor variables (Meng *et. al.,* 2013) (Table 3.2).

3.3.5. Grain Productivity and Topography

Pearson correlation (r) analysis showed weak correlation between grain productivity and a suite of terrain attributes for both sites (Table 3.4). These weak correlations could be explained by relatively uniform topography at both study sites. Therefore, topography might not subscribe as a strong propellant for grain productivity response. Given the weak correlations between soil fertility parameters and the evaluated terrain attributes (Table 3.2), this finding is perhaps not surprising. Slope (r = 0.20) and elevation (r = 0.13) were the best performing terrain attributes for the Bert and Lamoureux sites, respectively (Table 3.4), and this finding complied with earlier reports (Kaspar *et al.,* 2004, Kumhálová *et al.,* 2008). Slope and elevation affect physical and chemical soil properties through redistribution of soil as the result of erosion and deposition (Moulin *et al.,* 1994). Therefore, these topographic attributes generally perform well to predict grain productivity response across a landscape (Singh *et al.,* 2016). Weather conditions also affected the relationship between grain productivity and topography. Influence of topography on grain productivity appeared to be more pronounced during drier year i.e., 2015, in the study, and this finding was consistent with the conclusions drawn by Kumhálová *et al.* (2008). Drier weather conditions significantly influence the paradigm of water availability. Thus, the effect of topography on grain productivity is more prominent under such drier conditions.

3.3.6. Minimum Sample Size

Adequate sample size is an important pre-requisite for spatial modelling of a variable as it affects the reliability of the developed semi-variogram. Therefore, sample size is an important consideration in any sampling strategy. The size of samples required to estimate a given variable within 20% of the true value (N_{20}) offers a reasonable guide for designing future experiments for quantification of soil fertility parameters since this estimate is conservative enough to fulfill accuracy requirements (Loescher *et al.,* 2014), and also encompasses logistic feasibility. Sample size in our study, n = 79 for the Bert site, and n = 56 for the Lamoureux site, was adequate to quantify each soil fertility parameter with accuracy level of 20% and 50% of the true value, with the exception of AN at the Lamoureux site that required 76 samples for N_{20} at an alpha value of 5% (Table 3.7). There was a disparity between the ideal number of samples and the actual number of samples used to quantify certain variables (AN and OM at the Lamoureux site, and AP and AK at the Bert site) within 10% of the true value with alpha value of 5%, and this observation could be explained by high spatial variability (Metcalfe *et al.,* 2008), as given by their respective CV_{sill} (Table 3.7).

3.4. Conclusion

Although MLR analysis offers a good starting point to develop insight about correlations among data variables, it failed to capture the underlying spatial structure. In this study, the results from MLR analysis became of little practical significance. In general, OK was the best performing SIM for estimating soil nutrients in our study, as demonstrated by smaller values of error statistic, and RK outperformed OK and OCK for predicting pH, CEC, and OM. Even though OCK assimilated more auxiliary information related to terrain attributes in its prediction framework, it failed to deliver more accurate estimates in most cases. Therefore, landscape position was not strongly responsible for spatial heterogeneity in soil fertility parameters. Moreover, topography was not a strong driver of soil fertility and grain productivity.

3.5. Figures and Tables

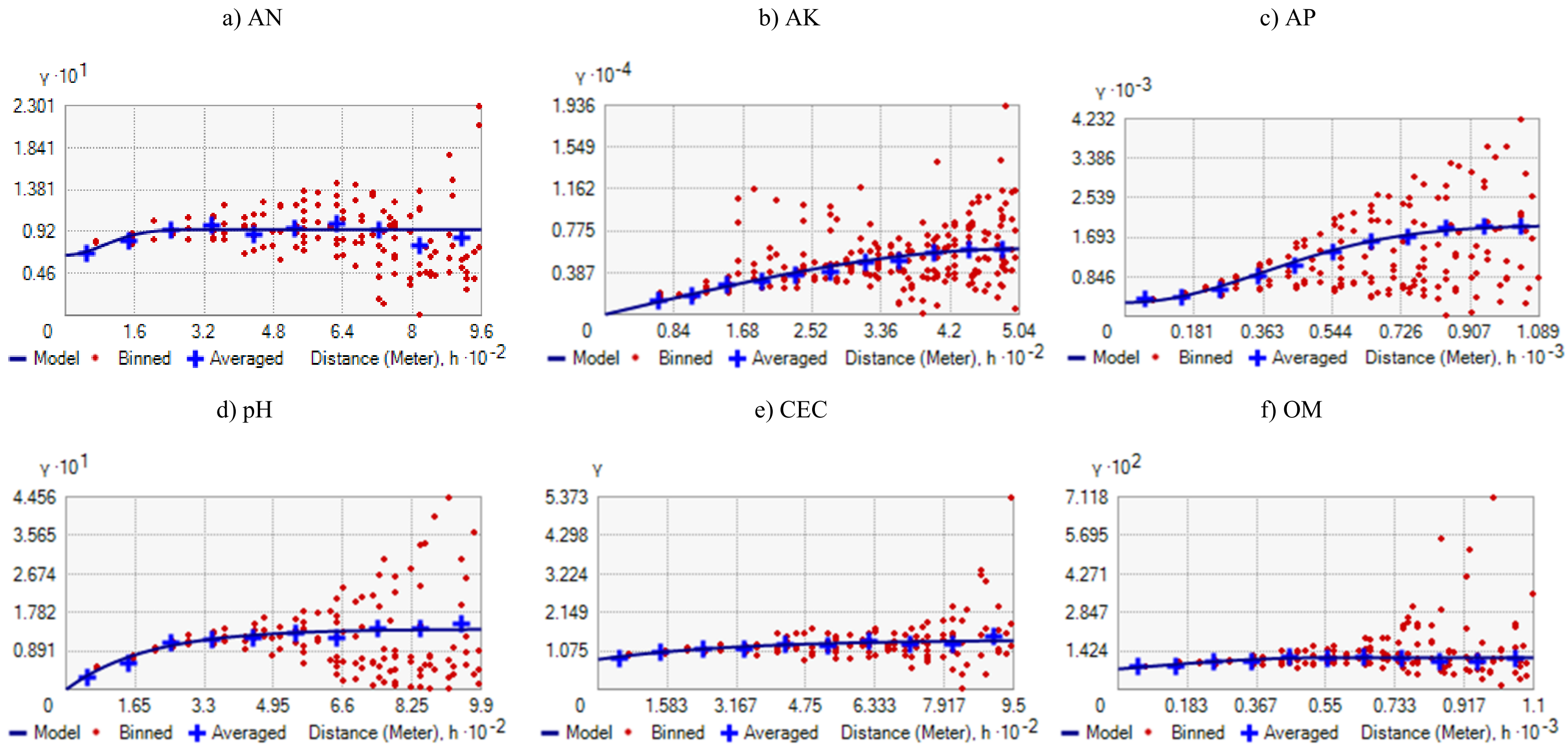

Figure 3.1. Semivariogram analysis of soil fertility parameters at the Bert site. Gaussian, spherical, or exponential model (as detailed in Table 3.5) were fitted to decipher spatial continuity of each variable of interest. AN: available soil nitrate (mg NO_3-N kg^{-1} soil); AK: readily available potassium (mg K_2O kg^{-1} soil); AP: readily available phosphorus (mg P_2O_5 kg^{-1} soil); CEC: cation exchange capacity (meq 100 g^{-1}); OM: organic matter (%).

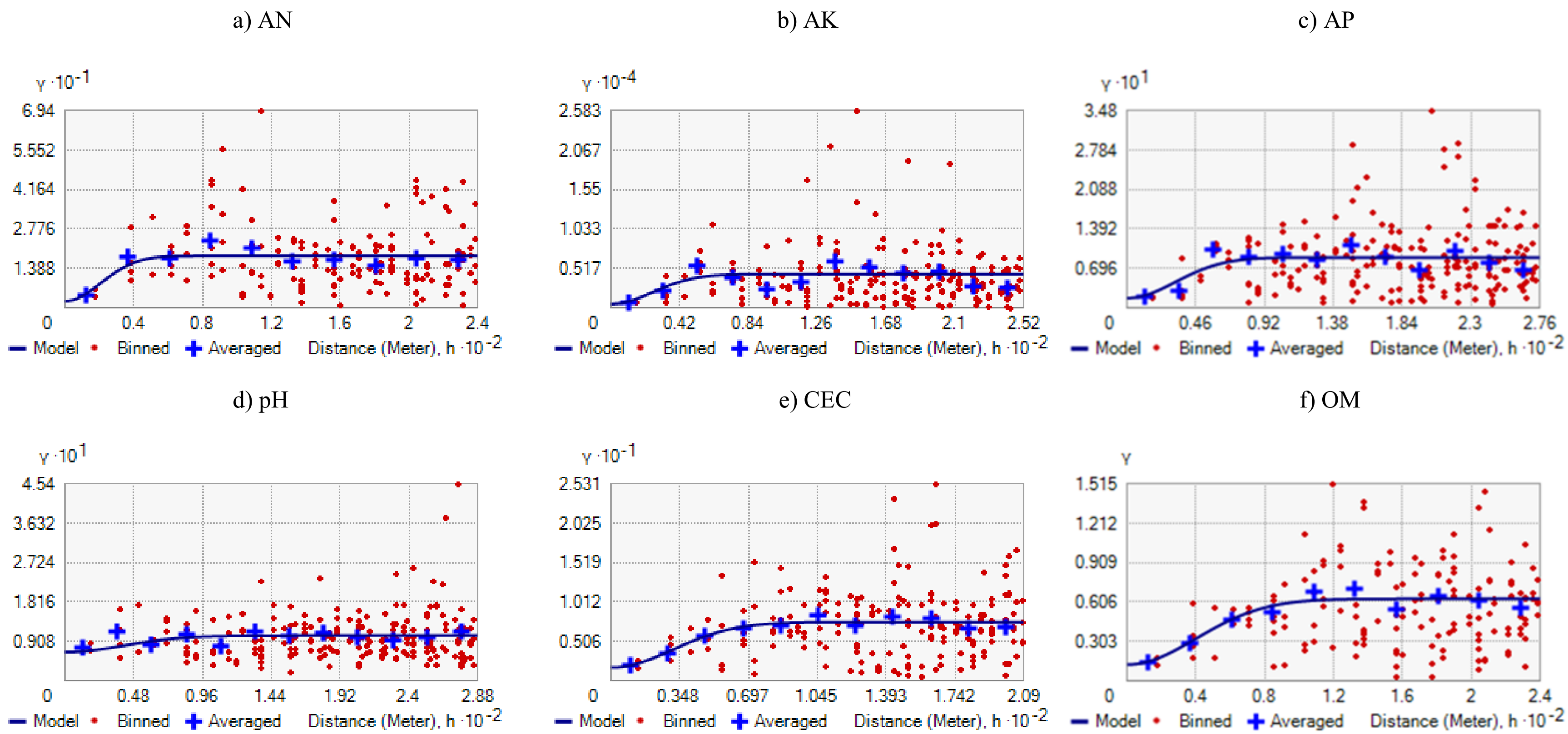

Figure 3.2. Semivariogram analysis of soil fertility parameters at the Lamoureux site. Spatial continuity of each soil fertility parameter was modelled as a function of distance using either gaussian, spherical, or exponential model (as detailed in Table 3.5). AN: available soil nitrate (mg NO_3-N kg^{-1} soil); AK: readily available potassium (mg K_2O kg^{-1} soil); AP: readily available phosphorus (mg P_2O_5 kg^{-1} soil); CEC: cation exchange capacity (meq 100 g^{-1}); OM: organic matter (%).

Table 3.1. Descriptive statistics of soil fertility parameters at a depth of 0-15cm and terrain attributes for the Bert (n = 79) and Lamoureux (n = 56) site.

Properties	**Type**	**Sites**	**Mean**	**SD**	**Min.**	**Max.**	**Skewness**	**Kurtosis**	**CV(%)**
AN (mg NO_3 -N kg^{-1} soil)	Response/ Predictor	Bert	15.91	4.77	7	29	0.66	0.34	30
		Lamoureux	6.79	4.74	1	16	0.39	-1.01	70
AK (mg K_2O kg^{-1} soil)	Response/ Predictor	Bert	223.7	84.58	55	422	-0.06	-0.32	38
		Lamoureux	288.2	92.80	126	508	0.38	-0.60	32
AP (mg P_2O_5 kg^{-1} soil)	Response/ Predictor	Bert	77.46	34.41	4	149	-0.33	-0.96	44
		Lamoureux	28.98	16.95	11	98	1.80	3.76	58
pH	Response/ Predictor	Bert	5.21	0.56	4.30	8.10	2.60	9.39	11
		Lamoureux	5.8	0.80	5.1	7.8	1.60	1.07	14
CEC (meq 100 g^{-1})	Response/ Predictor	Bert	15.43	2.93	7.4	24.8	-0.37	1.41	19
		Lamoureux	15.81	4.43	7.9	25.20	0.53	-0.48	28
OM (%)	Response/ Predictor	Bert	4.16	1.10	1.6	8.7	0.77	2.83	26
		Lamoureux	4.96	1.03	3.4	7.2	0.60	-0.74	21
Extractable Magnesium	Predictor	Bert	135.6	42.38	50	241	0.38	-0.20	31

(ppm)		Lamoureux	165.1	83.80	70	340	0.94	-0.56	50
Extractable Manganese	Predictor	Bert	28.24	12.64	4	56	0.23	-0.64	45
(ppm)		Lamoureux	15.48	11.45	ND	71	2.33	9.18	74
Extractable Copper	Predictor	Bert	1.20	0.53	0.5	4.1	2.36	9.33	44
(ppm)		Lamoureux	0.47	0.21	ND	1.40	1.89	5.99	45
Extractable Boron (ppm)	Predictor	Bert	0.62	0.32	0.3	1.8	1.7	5.7	52
		Lamoureux	0.65	0.36	ND	1.70	1.57	1.77	55
Extractable Iron (ppm)	Predictor	Bert	233.8	221.07	44	999	2.19	4.13	95
		Lamoureux	135.6	83.77	ND	378	0.84	0.44	62
Extractable Zinc (ppm)	Predictor	Bert	3.38	1.28	1.20	8.90	1.30	3.18	38
		Lamoureux	1.26	0.92	ND	5.2	2.21	5.96	73
Elevation	Covariate	Bert	658.34	2.97	648	662	-2.70	9.93	0.45
(m)		Lamoureux	647.12	2.87	645	651	0.61	1.38	0.44
Slope (°)	Covariate	Bert	25.13	17.84	0	85	0.25	2.66	71
		Lamoureux	38.59	13.33	3.04	76.16	0.15	2.40	34
Curvature	Covariate	Bert	-0.27	46.68	-183.1	287	-0.57	30.44	–

(m^{-1})		Lamoureux	-0.01	42.77	-225	212.5	-0.07	3.27	–
Aspect	Covariate	Bert	146.98	105.78	0	358.71	0.01	1.84	72
(m)		Lamoureux	189.15	82.65	0.95	354.6	0.04	2.07	44
Hillshade	Covariate	Bert	118.71	88.16	0	254	-0.15	1.53	74
(°)		Lamoureux	141.82	80.40	0	254	-0.37	1.83	57

AN: available soil nitrate (mg NO_3-N kg^{-1} soil); AK: readily available potassium (mg K_2O kg^{-1} soil); AP: readily available phosphorus (mg P_2O_5 kg^{-1} soil); CEC: cation exchange capacity (meq 100 g^{-1}); OM: organic matter (%), ND: not detected.

Table 3.2. Pearson correlation of soil fertility parameters with auxiliary variables and terrain covariates. Soil fertility analysis was conducted on spring soil samples collected at a depth of 0-15 cm from the Bert and Lamoureux site. Terrain covariates were extracted from topographic LIDAR data collected using ArcGIS.

Site	**Soil property**	**Mg**	**Mn**	**Cu**	**B**	**Fe**	**Zn**	**Elevation**	**Slope**	**Curvature**	**Aspect**	**Hillshade**
Bert	AN	0.00	0.33**	0.19	0.11	0.29**	0.28*	0.04	0.04	-0.09	-0.05	-0.16
	AK	-0.03	0.21	0.21	-0.33**	0.01	0.33**	-0.05	0.21	-0.02	-0.04	0.07
	AP	-0.15	0.20	0.22*	-0.30**	0.06	0.42***	-0.14	0.28*	-0.07	-0.10	-0.03
	pH	0.73***	-0.64***	-0.31**	0.36**	-0.31**	-0.28	-0.07	-0.26	0.07	0.07	0.12
	CEC	0.77***	-0.11	-0.05	0.35	-0.10	-0.00	0.11	-0.21	0.09	0.02	0.10
	OM	-0.13***	0.46**	-0.19	0.40**	0.32	0.03	0.05	-0.17	0.06	0.04	0.07
Lamoureux	AN	-0.30*	0.01	0.13	-0.27	0.45**	0.30*	-0.13	-0.32*	-0.06	-0.04	0.09
	AK	-0.71***	0.12	0.22	-0.51***	0.68***	0.42**	-0.09	0.13	0.03	0.07	0.29*
	AP	-0.62***	-0.02	0.07	-0.48***	0.46***	0.32*	0.31*	0.16	-0.14	-0.32*	0.40**
	pH	0.87***	-0.50***	0.01	0.91***	-0.53***	-0.05	0.28*	-0.07	-0.01	0.12	-0.07
	CEC	0.90***	-0.37**	-0.03	0.82***	-0.55***	-0.14	0.01	0.14	-0.10	-0.04	-0.14

OM	0.60***	-0.29*	0.11	0.67	-0.26	0.19	0.04	-0.02	0.17	0.09	0.11

AN: available soil nitrate (mg NO_3-N kg^{-1} soil); AK: readily available potassium (mg K_2O kg^{-1} soil); AP: readily available phosphorus (mg P_2O_5 kg^{-1} soil); CEC: cation exchange capacity (meq 100 g^{-1}); OM: organic matter (%), Mg: Magnesium (ppm), Mn: Manganese (ppm), Cu: Copper (ppm), B: Boron (ppm), Fe: Iron (ppm), Zn: Zinc (ppm).

*indicates p-value < 0.05, ** indicates p-value < 0.01, *** indicates p-value < 0.001

Table 3.3. Step-wise multiple linear regression analysis of different soil fertility parameters at the Bert and Lamoureux site.

Site	Soil property	Regression equation	R^2
Bert (n = 79)	AN[a] (mg NO_3-N kg^{-1} soil)	2.31 + 0.03 (CEC)	0.05
	AK (mg K_2O kg^{-1} soil)	492.64 – 51.57 (pH)	0.10
	AP (mg P_2O_5 kg^{-1} soil)	209.98 – 25.41 (pH)	0.16
	pH	4.71 + 0.01 (Mg) – 0.02 (Mn)	0.61
	CEC (meq 100 g^{-1})	2.09 + 8.63 (log OM) + 0.01 (Mg)	0.85
	OM[a] (%)	– 0.12 + 0.08 (CEC) + 0.05(pH)	0.85
Lamoureux (n = 56)	AN (mg NO_3-N kg^{-1} soil)	15.49 – 2.13 (pH) + 0.11 (slope)	0.20
	AK (mg K_2O kg^{-1} soil)	643.61 – 61.24 (pH)	0.27
	AP[a] (mg P_2O_5 kg^{-1} soil)	– 0.80 – 0.41 (pH) + 0.03 (elevation)	0.44
	pH	– 1.47 + 0.12 (CEC) + 0.67 (log OM) – 0.09 (AN) + 0.02 (elevation)	0.83
	CEC (meq 100 g^{-1})	– 14.57 + 10.11 (log OM) + 2.48 (pH)	0.64
	OM[a] (%)	2.25 + 0.17 (CEC)	0.54

AN: available soil nitrate (mg NO_3-N kg^{-1} soil); AK: readily available potassium (mg K_2O kg^{-1} soil); AP: readily available phosphorus (mg P_2O_5 kg^{-1} soil); CEC: cation exchange capacity (meq 100 g^{-1}); OM: organic matter (%); Mg: Magnesium (ppm), Mn: Manganese (ppm)

[a] based on log-transformed data

Table 3.4. Pearson correlation of grain yield (kg ha^{-1}) with terrain covariates. Grain yield data were recorded in 2015 at the Bert and 2017 at the Lamoureux site, using Green Star Monitor 3 mounted combine harvester. Terrain covariates were acquired from airborne LIDAR topographic data extracted using ArcGIS ver. 10.5.1 (ESRI, Redlands, CA, USA).

Site	Year	AnP (mm)	Elevation	Slope	Curvature	Aspect	Hillshade
Bert (n = 43258)	2015	357	0.18***	0.20***	0.18***	0.19***	0.19***
Lamoureux (n = 30439)	2017	328	0.13***	0.02***	0.01	0.10***	0.11***

*** indicates p-value < 0.001

AnP: Annual precipitation (mm)

Table 3.5. Semivariogram analysis for the optimal geostatistical methods for the given soil fertility parameters at the Bert and Lamoureux sites.

Site	Soil property	Geostatistical method	Covariate	Model	Range (m)	Nugget (C_o)	Partial Sill (C)	Sill (C_o + C)	Nugget-to-sill ratio	Spatial dependence
Lamoureux	**AN**	Regression kriging	N/A	Gaussian[a]	50.39	2.39	15.89	18.28	0.13	Strong
Bert	**AN**	Ordinary kriging	N/A	Gaussian[a]	218.70	0.07	0.03	0.09	0.77	Weak
Bert	**AP**	Ordinary kriging	N/A	Gaussian[a]	889.69	295.83	1653.88	1949.71	0.15	Strong
Lamoureux	**AP**	Ordinary kriging	N/A	Gaussian[a]	78.81	0.02	0.07	0.09	0.22	Strong
Bert	**AK**	Ordinary kriging	N/A	Spherical[a]	504	3.36	6068.28	6071.64	0.00	Strong
Lamoureux	**AK**	Ordinary kriging	N/A	Gaussian[a]	62.30	520.56	3903.13	4423.69	0.12	Strong
Bert	**CEC**	Regression kriging	N/A	Exponential[a]	950	0.84	0.55	1.39	0.60	Moderate
Lamoureux	**CEC**	Regression kriging	N/A	Gaussian[a]	76.61	1.70	5.85	7.55	0.22	Strong
Bert	**pH**	Regression kriging	N/A	Exponential[a]	579.97	0.00	0.14	0.14	0.00	Strong
Lamoureux	**pH**	Regression kriging	N/A	Gaussian[a]	100.68	0.07	0.04	0.11	0.64	Moderate
Bert	**OM**	Regression kriging	N/A	Spherical[a]	536.28	0.01	0.00	0.01	1	Weak
Lamoureux	**OM**	Regression kriging	N/A	Gaussian[a]	97.72	0.16	0.50	0.66	0.24	Strong

AN: available soil nitrate (mg NO_3-N kg^{-1} soil); AK: readily available potassium (mg K_2O kg^{-1} soil); AP: readily available phosphorus (mg P_2O_5 kg^{-1} soil); CEC: cation exchange capacity (meq 100 g^{-1}); OM: organic matter (%); [a] based on isotropic model.

Table 3.6. Performance assessment of different non-geostatistical and geo-statistical spatial interpolation methods used to quantify each soil fertility parameter at the Bert and Lamoureux sites.

Soil Property	**Site**	**Multiple linear regression (MLR)**			**Ordinary kriging (OK)**			**Ordinary cokriging (OCK)**			**Regression kriging (RK)**		
		RMSE	**MSE**	**MAE**	**RMSE**	**MSE**	**MAE**	**RMSE**	**MSE**	**MAE**	**RMSE**	**MSE**	**MAE**
AN	Lamoureux	4.12	16.98	3.41	3.01	9.06	2.18	3.58	12.83	2.69	3.58	12.87	2.67
	Bert[a]	0.29	0.08	0.23	4.57	20.93	3.52	4.59	21.13	3.53	0.26	0.07	0.20
AK	Lamoureux	77.94	6074.72	60.90	68.82	4735.67	50.30	74.40	5535.22	53.48	76.08	5788.91	56.34
	Bert	79.02	6244.73	63.33	41.38	1712.58	33.46	42.09	1771.31	33.70	47.68	2273.33	35.88
AP	Lamoureux[a]	0.36	0.13	0.27	12.95	167.77	8.11	13.76	189.44	8.38	0.35	0.12	0.25
	Bert	30.54	932.72	26.14	18.60	346.28	14.94	18.05	325.82	14.17	19.46	378.60	15.62
pH	Lamoureux	0.31	0.10	0.26	0.37	0.14	0.28	0.44	0.19	0.33	0.30	0.09	0.24
	Bert	0.34	0.11	0.22	0.33	0.11	0.20	0.32	0.10	0.22	0.22	0.05	0.14
CEC	Lamoureux	2.58	6.67	2.08	2.25	5.07	1.59	2.93	8.57	2.41	2.12	4.49	1.63
	Bert	1.11	1.24	0.91	2.66	7.11	2.01	2.70	7.27	2.07	1.10	1.22	1.22
OM	Lamoureux[a]	0.68	0.47	0.54	0.76	0.58	0.57	0.70	0.50	0.52	0.64	0.41	0.48
	Bert[a]	0.11	0.01	0.08	0.90	0.81	0.65	0.93	0.86	0.69	0.10	0.01	0.08

AN: available soil nitrate (mg NO_3-N kg^{-1} soil); AK: readily available potassium (mg K_2O kg^{-1} soil); AP: readily available phosphorus (mg P_2O_5 kg^{-1} soil); CEC: cation exchange capacity (meq 100 g^{-1}); OM: organic matter (%); RMSE: root mean square error; MSE: mean square error; MAE: mean absolute error; [a]based on log-transformed data.

Table 3.7. Sample size to estimate soil fertility parameters with given accuracy of 10%, 20% or 50% of the true value at an alpha value of 0.05 and 0.1. These calculations are based on CV_{sill} which is a measure of spatial variability in overall data.

Site	Soil property	CV_{sill}	Sample size					
			$\alpha = 0.05$			$\alpha = 0.1$		
			N_{10}	N_{20}	N_{50}	N_{10}	N_{20}	N_{50}
Bert	AN	0.16	10	3	0	7	2	0
	AK	0.49	93	23	4	66	16	3
	AP	0.80	250	62	10	176	44	7
	pH	0.10	4	1	0	3	1	0
	CEC	0.10	5	1	0	3	1	0
	OM	0.10	4	1	0	3	1	0
Lamoureux	AN	0.89	305	76	12	215	54	9
	AK	0.32	41	10	2	29	7	1
	AP	0.13	7	2	0	5	1	0
	pH	0.08	3	1	0	2	0	0
	CEC	0.24	23	6	1	16	4	1

OM	0.71	194	49	8	137	34	6

AN: available soil nitrate (mg NO_3-N kg^{-1} soil); AK: readily available potassium (mg K_2O kg^{-1} soil); AP: readily available phosphorus (mg P_2O_5 kg^{-1} soil); CEC: cation exchange capacity (meq 100 g^{-1}); OM: organic matter (%). N_{10} = sample size to estimate a given measurement within 10% of the true value; N_{20} = sample size to estimate a given measurement within 20% of the true value; N_{50} = sample size to estimate a given measurement within 50% of the true value.

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Conclusion

Agriculture is a major contributor of green house gas emissions. Excessive application of nitrogenous fertilizers results in nitrous oxide (N_2O) emissions, and given the high global warming potential, these N_2O emissions are detrimental to environmental health and sustainability. Therefore, it is becoming crucial to improve the efficiency of cropping systems. Finding concurrent solution to food security and environmental sustainability is pivotal to mitigate climate change driven by intensive agriculture. Precision agriculture (PA) offers a plausible solution to two contrasting challenges faced by the modern agriculture—food security and sustainable environment. It promises the possibility of sustainable food production while managing the impact of anthropogenic hazards on environment.

Success of PA technology hinges on a sound knowledge of the field and prudent management decisions. It is also imperative to make timely decisions given the weather conditions. Quantifying in-field yield variability is crucial to its precise management. Yield maps generate historic footprint of yield variability for a given field, and data from at least 3-5 previous years offers a good starting point for farmers to start understanding in-field yield variability prevalent at their farms. Farmers can divide their fields into different productivity zones (i.e., low, medium, and high). Based on this understanding of their field, farmers can make prudent management decisions to increase their economic return while mitigating global ecological footprint. Economic benefits of yield map-based management can be observed by considering the following examples. Suppose a 100 hectares of wheat field, and 15% of this farm was heavy clay soil. Let's say, for 2017, the early growing season was wet, and almost half of the applied N to this patch of land was leached below the root zone, and therefore, became unavailable to the plants. This developing N stress was detected through crop scouting. A second doze of N was applied to this patch of land, and this helped farmer to avoid potential yield losses. A simple calculation can help us understand the profitability of PA adoption in this case. For example, if yield recovery was 50% of the average 1500 kg ha^{-1}, and the second application of N would have increased 11250 kg (750 kg ha^{-1} x 15 ha) of yield. At \$0.25 kg^{-1}, there would have been an economic gain of \$2812.5 on 100 hectares farm. There is also a possibility that similar economic gains might not be extended to severely water-logged area in a farm, and farmer might deem this area unfit for cultivation in the coming years. In such a scenario, the farmer not only achieves sustainability goal of PA technology, but is also able to ration his resources to where they are needed, thus improving his economic benefits.

Consider another example to examine the economic benefits of PA technology. A Canadian farmer fertilized his 50 hectares farm with a uniform rate of 220 kg ha^{-1} with a total N fertilizer cost of \$13,200 (plus cost of application, including machinery and labour). Comprehensive assessment of spatio-temporal variability of available soil N showed that the farm could be delineated into 3 N management zones: 15 hectares of 140 kg ha^{-1}, 25 hectares of 190 kg ha^{-1}, and 10 hectares 200 kg ha^{-1} of urea (46-0-0). In this example, dividing the field into 3 management zones reduced N fertilizer cost to \$10,620 for 50 hectares. In addition to increased profitability, environmental sustainability was also improved by matching N fertilizer rate to the crop requirement.

"Garbage In, Garbage Out"— being a big data science, PA is also subjected to this limitation. Collection of meaningful datasets is more important than collecting big datasets. Farmers might feel overwhelm with the amount of data generated in a short period of time, and may fail to capitalize on the amount of information available. Practical implementation of the developed solutions imposes a hurdle to realize the full potential of PA technology.

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