Modelling regional land use

The quest for the appropriate method

Afsaneh Soltani Largani

Thesis committee

Promotor
Prof. dr. ir. A. Veldkamp
Professor of Land Dynamics
Wageningen University

co-promotor
Dr. M.M. Bakker
Associate professor, Land Use Planning Group
Wageningen University

Dr. Ir. J.J. Stoorvogel
Associate professor, Soil Geography and Landscape Group
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Afsaneh Soltani Largani

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Afsaneh Soltani Largani

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1 Introduction

1.1 Legitimacy

According to the latest revision of the UN population prospects (UN, 2010), the world population is projected to grow by 32 percent from 6.9 billion in 2010 to 9.1 billion in 2050. To meet the demand for food, annual grain production will need to rise from 2.2 billion ton in 2010 to about 3.0 billion ton in 2050 (FAO, 2010). In addition, the threat of regional imbalances in food supply and demand will continue to rise as crop production faces the challenges of climate change, limited and dwindling resources, and increasing energy needs and prices. Many national and international organizations aim to minimize this threat, and safeguard a sustainable use of natural resources (GECATS, 2012; Justice and Becker-Reshef, 2007; IGOL, 2006; Becker-Platen, 1979). Timely and accurate information on spatial patterns of crop yield is important for commercial interests (Jagtap and Jones, 2002), strategic agricultural planning (Lobell and Ortiz-Monasterio, 2007), public policy formulation and application (De Wit et al., 2005; Wassenaar et al., 1999), and agricultural scientific innovation (Williams et al., 2008). This includes information on current crop-yield patterns as well as explorations of future scenarios (e.g. climate change).

1.2 Overview of methodological approaches in crop yield estimates studies

Probably the most widely used technique to assess the spatial patterns of crop yield is by means of the agricultural census or other forms of surveys (Dobermann et al., 2003; Downing et al., 1999). Alternatively, remote sensing techniques have shown to be effective in mapping regional patterns of crop yield and in monitoring changes at regular intervals (Khan et al., 2010; Launay and Guerif, 2005). The main limitation of these assessments is that they only provide insight *ex post*. Therefore, there is a continuing need for the development of modelling approaches to assess a priori and/or future (*ex ante*) ranges of alternative scenarios for the spatial patterns of crop yield. Ideally, a generic crop growth simulation model (CGSM) would be developed for the regional level which would be fed with high-resolution input data on weather, soil, and management data so as to provide accurate regional patterns of crop yield. Currently, CGSMs are able to integrate the effects of agricultural management under a wide range of climatic and soil conditions and offer good insight in the spatial variability of crop yield at the field level (e.g. Xiong et al., 2008; Launay and Guérif, 2003; Faivre et al., 2000). In the past forty years, different CGSMs have been developed to serve a variety of applications (Matthews and Stephens, 2002). DSSAT (Decision Support System for Agro-technology Transfer) was developed in the USA by IBSNAT (International Benchmark Sites Network for Agro-technology Transfer) (Jones et al., 2003). The APSIM (Agricultural Production system SIMulator) modelling framework was developed by APSRU (Agricultural Production Systems Research Unit) in Australia (Thorburn et al., 2010; Keating et al., 2003). In the Netherlands, de Wit started working on crop growth simulation modelling at the Department of Theoretical Production Ecology of Wageningen Agricultural University (Van Keulen et al., 2008; Van Ittersum et al., 2003). Although CGSMs aim to be universal (within certain boundary conditions), they still require calibration for prediction outside the observed data range or in extreme environmental situations, a CGSM might have to be redeveloped or calibrated to produce useful results (Wang et al., 2002; Basso et al., 2001; Bolte, 1997).

Despite all the efforts, CGSMs are not available for all cropping systems. For example, there are still many perennial crops (e.g. coffee, tea, and banana) for which no CGSMs have been developed (Zuidema et al., 2005). In addition, there is still a lack of models that can handle the impact of weeds, micro nutrients, and mixed cropping. Moreover, many CGSMs have been designed to simulate crop production for a field, while no process-based simulation models are specifically developed to assess regional patterns of crop yield. The development of such regional models is troubled by the lack of insight in processes specific to the regional level (Veldkamp et al., 2001). The calibration and application of regional models is furthermore hampered by the data requirements of such models.

1.3 Application of crop growth simulation models at the regional level

Due to the urgent call from policymakers for methods to assess regional patterns of crop yield, scientists pragmatically used field-level CGSMs at regional scales (e.g. Xiong et al., 2008; Launay and Guérif, 2003; Faivre et al., 2000). Such applications aim to identify (i) the effect of climate change (e.g. Reidsma et al., 2009; Hansen and Jones, 2000), (ii) the impact of changes in land use, policy and technology (e.g. Godard et al., 2008), and/or (iii) annual yield forecasts (e.g. Yun, 2003; Jagtap and Jones, 2002; Supit, 1997). However, two main problems emerge in the application of field-level CGSMs at regional scales. Firstly, the required input data on weather, soils, and management are often not available (data availability); and secondly, if they are, generally not at the required level of detail (data aggregation).

1.3.1 Data availability

Increasing the extent from a homogeneous field to regional level requires incorporating additional spatial variability of the input data (Faivre et al., 2004; Hansen and Jones, 2000). This is because by increasing the extent of the study area, new variability of input data emerges. For instance, soil varies in depth, texture, and chemical properties; climate, in particular rainfall, becomes more variable; and so do management practices (soil tillage, irrigation, fertilization, choice of cultivar, etc.). The availability of data on weather, soil, and management is one of the problems faced by the application of the models at the regional level (Carbone et al., 2003; De Bie, 2000; Nachtergaele, 2000; Fresco et al., 1997; Sombroek and Antoine, 1994). Although there are many approaches developed to generate input data (e.g. Leenhardt et al., 2006; Launay, 2002; Heinemann et al., 2002; Voltz and Webster, 1990; Webster and Beckett, 1968), the criteria for selecting the best approach are often unclear. Moreover, using these approaches to generate input data may have implications for model outcomes. One could argue that empirical models with lower input data requirements, in which historical data on crop yields and predictors are used to calibrate relatively simple regression equations, provide a useful alternative to CGSMs (see e.g. De Vries et al., 1998; Beven, 1989).

1.3.2 Data aggregation

CGSMs are mainly developed for the plot and field scale, requiring location-specific, spatially homogenous input data (Tao et al., 2009; De Wit et al., 2005; Van Ittersum et al., 2003; Mearns et al., 2001; Hansen and Jones, 2000). The availability of such data is one of the problems faced by the application of the models at the regional level (Carbone et al., 2003; De Bie, 2000; Nachtergaele, 2000; Fresco et al., 1997; Sombroek and Antoine, 1994). Soil and daily climate data are often available from existing databases at different spatial levels of detail, but spatially and temporally explicit information on crop management is much less readily available (Leenhardt et al., 2010; Godard et al., 2008; Maton et al., 2007; Mignolet et al., 2007; Faivre et al., 2004; Biarnès et al., 2004; Jagtap and Jones, 2002). Therefore, in contrast to field-scale model applications, regional-scale applications often rely on data aggregated over space and/ or time. In general, with increasing aggregation (i.e. an increase in support) variability of data will decrease and local extremes will be levelled out (Baron et al., 2005: Hansen and Ines, 2005; Easterling et al., 1998). Depending on the spatial distribution, this effect will be stronger for some variables than for others. As a result, quantitative relationships between variables may change with aggregation. Using aggregated input data requires therefore recalibration of the models. Also when relationships are non-linear, aggregation will have implications for model outcomes (Ewert, 2004). A sensitivity analysis is a suitable methodology to identify the degree to which input variables are affected by aggregation, and can therefore be used to study if aggregation of specific input data is appropriate (Hansen and Jones, 2000). Furthermore, a sensitivity analysis of the extent to which the variables of a chosen model will influence model output and accuracy, may identify the most significant/relevant input variables of the model in response to specific output (e.g. yield). This allows focusing data collection efforts on these particular variables.

Apart from adjusting the CGSM to regional scale and/or generating the required detailed input data, there are two other known solutions for solving the scaling issue. One is replacing the CGSM by a metamodel that can deal with less detailed data (Kleijnen and Sargent, 2000; Barton, 1998), and the second approach is using the less detailed data to derive a simple empirical model (Lobell and Burke, 2010; White, 2009; Veldkamp et al., 2001). Initially, a metamodel requires similar data as the original process-based CGSM for its development, although these data may be up-scaled to more practical temporal and spatial resolutions (Audsley et al., 2008). Metamodels are relatively simple, can easily be applied by end users such as policymakers, and require less data for their application compared to the CGSM (Kleijnen and Sargent, 2000; Barton, 1998). However, as such a metamodel is based on the CGSM, the problem of not including factors (Donatelli et al., 2010) that play a role at wider temporal and spatial scales may not be solved.

An empirical model can use all data available including other data sources depending on availability and hypothesized relationships. It is calibrated directly on the aggregated input data, and can include all kinds of factors at any available aggregation level (see e.g. De Vries et al., 1998; Beven, 1989). Empirical models are able to represent factors that are not present in CGSMs, such as proxies for the occurrence of pests and diseases. The advantages of the empirical models furthermore concern their ease to be used by a broad group of users with limited process knowledge. Due to the lower data requirements, errors associated with uncertainties in input data are smaller. However, disadvantages of metamodels and empirical models are that extrapolation beyond the calibration range of input variables is unreliable, and the relationships that comprise the model are context dependent and not process-based (Bakker and Veldkamp, 2012). Furthermore, aggregation of spatial data may lead to linearization of relationships obscuring the underlying complexity (Kok and Veldkamp, 2011).

1.4 Scope and objectives

This study is mainly concerned with how to model spatial patterns of crop yield at the regional scale. The definition of regional scale varies with different settings. In this study I adopt an operational definition in which the regional level includes the scale levels above the field level (i.e. for which it is impossible to deal with individual fields) up to the national level. In practice this means that I deal with a population of farms or fields (survey data) or administrative regions (agricultural statistics). Applying and developing models at the regional scale has various consequences. Scale is defined on the basis of extent (i.e. the spatial area covered by the simulation), support (i.e. the spatial area covered by the observed data), and resolution (i.e. the ratio between the support and the extent) (e.g. Bierkens et al., 2000; Faivre et al., 2004). As soon as we move towards higher scale levels the extent increases. By increasing the extent of the study, new processes and variables possibly emerge as driving factors behind the variability in crop yield. For example, spatial variability of access to markets can emerge as a determinant of spatial patterns, or a regional variability in sensitivity to plagues and diseases may appear. Thus, with increasing extent it becomes necessary to incorporate additional data (Faivre et al., 2004; Hansen and Jones, 2000). The higher scale level also means that data on weather, soils, and management are not available at the same resolution. While detailed soil maps may be available at a scale of 1:20,000 for small areas, regional exploratory surveys are typically at a scale of 1:50,000 to 1:250,000.

In this thesis, different modelling approaches will be used to model regional patterns of crop yield for cases in which:

- Survey data of yield and its predictors (e.g. soil, weather conditions) are available; data will be used to develop an empirical model to model the spatial patterns of crop yield.
- The availability of a calibrated CGSM allows us modelling the spatial patterns of crop yield with the environmental data.
- A metamodel will be constructed by identifying the most significant input variables of the calibrated CGSM in response to crop yield.

Three different modelling approaches, being empirical models, CGSMs, and metamodels of the CGSMs, were distinguished to simulate regional patterns of crop yield. The context conditions that determine the best approach are input data requirements, problem definition, study sub-objective, the scale at which results are expected, model end-users, and utilization of the output (e.g. testing different scenarios). Which modelling-approach to choose, and how the model will eventually perform, is context dependent.

Context means the specific properties of the region, the data availability in that region, and for what purpose the model will be used.
Since there will always be a certain level of idiosyncrasy to the case, one has to strive for a toolbox of approaches from which the proper tool can be selected on the basis of a number of specific criteria such as credibility and sensitivity. Models are typically evaluated in terms of their credibility in modelling yield patterns, on the basis of a range of observation points using statistical techniques like the root mean square difference (Akinbile and Yusoff, 2011; Quiroga and Iglesias, 2009; Xiong et al., 2008). For the application of a model to a specific area and period, verifying its sensitivity to variables that are known to play an important role in that area and period is also essential. When the model itself is to be run by policymakers, user-friendliness is also an important criterion.

The selection of the modelling approaches can be considered as one of the most difficult, and often ignored, steps to model crop yield at the regional level. However, a structured, systematic way of modelling-approach selection is lacking. In order to address this issue I aimed to develop a framework for recommendable practices to model regional patterns of crop yield. From this general objective, more specific sub-objectives are derived:

- To provide decision rules for selecting appropriate approaches to generate input variables to feed crop growth simulation models at the regional level;
- To provide decision rules for selecting appropriate procedure s to simulate regional yield patterns using CGSMs;
- To identify, given context conditions, the most suitable modelling approach to simulate regional patterns of crop yield.

1.5 Outline of the thesis

To develop a framework for recommendable practices to model regional patterns of crop yield, in this thesis I explore proper input data for modelling, model implementation, and model selection criteria (Figure 1-1).

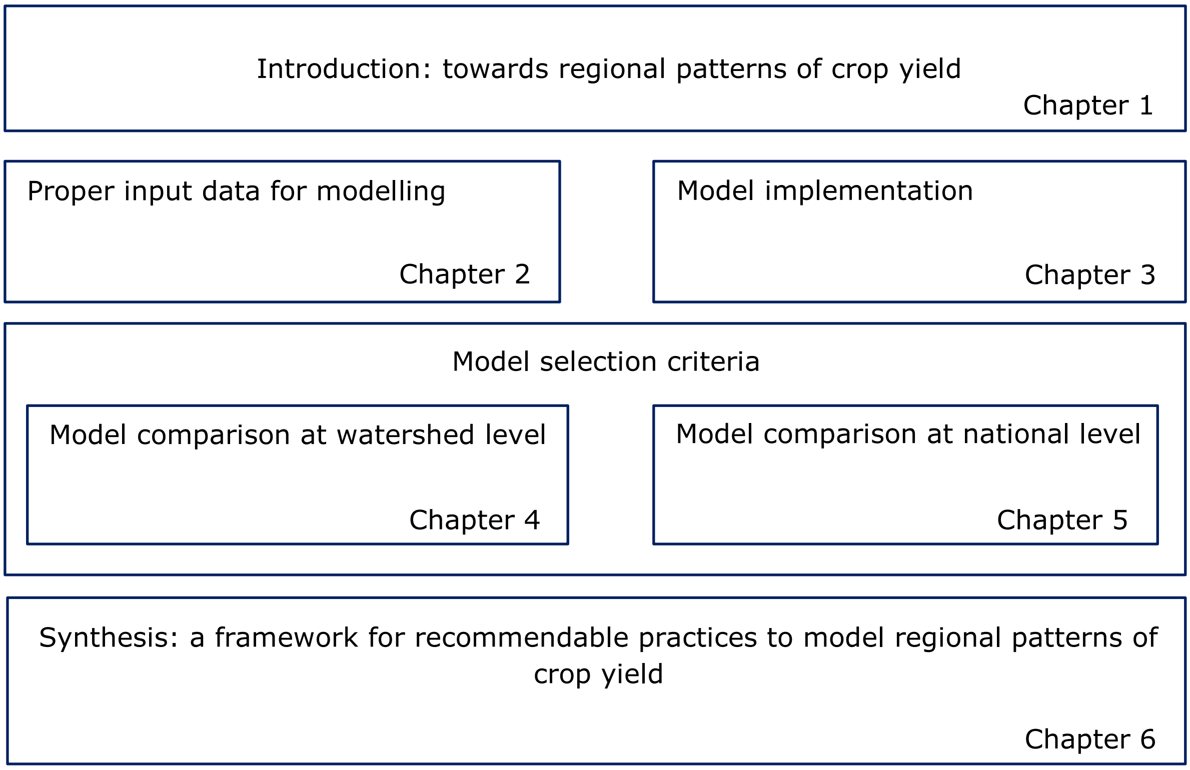

Figure 1-1: the contribution of this thesis to the development of a framework for recommendable practices to model regional patterns of crop yield consists of (i) proper input data for modelling, (ii) model implementation, and (iii) model selection criteria.

In Chapter 2, the issue of data availability is discussed, literature is reviewed for existing approaches that have been used to overcome the problem of data availability, and decision rules for selecting appropriate approaches to supply CGSMs at the regional level with suitable weather, soil, and management data are proposed. It starts by discussing the three main domains of input data by looking at the spatial characteristics of the variable, the availability of data at the regional level, and reviewing the approaches that people have been using to generate input data for CGSM applications at the regional level. Then, it focuses on the opportunities created by new interpolation techniques and the use of auxiliary data. Finally, the review is used to formulate decision rules as to when to use which approach.

Chapter 3 evaluates and selects different procedures for CGSM implementation to simulate regional yield patterns for a specific situation. The approaches include (i) run the CGSMs for a series of points distributed throughout a region after which the simulated crop productions can be interpolated to create a continuous surface of yield patterns, and (ii) create surfaces for each of the input variables individually, and then run the CGSM for each location (grid cell) to create a continuous surface of yield patterns. Moreover, scaling effects of different supports by aggregating either input or output at different spatial resolutions are examined. These procedures are applied to a complex CGSM (SUBSTOR-potato model, Ritchie et al., 1995) for the potato-pasture production system in the Carchi province in Northern Ecuador.

Choosing the most appropriate modelling approach should happen in terms of various criteria. Different modelling approaches to model regional patterns of crop yield including empirical models, CGSMs, and metamodels of the CGSMs are selected. Chapters 4 and 5 compare and evaluate the performance of three different modelling approaches for their capacity to model regional patterns of crop yield for two different regions: the Carchi province in Northern Ecuador (Chapter 4) and Western Germany (Chapter 5). For the Carchi study area, spatial analyses were carried out at watershed level, while for Western Germany spatial and temporal analyses were carried out at national level. The CGSM used for the Carchi study area was the SUBSTOR-potato model (Ritchie et al., 1995); the CGSM used for Western Germany was the LINTUL2 model (van Ittersum et al., 2003). The main strengths and limitations of the modelling approaches are discussed. Based on these findings, various criteria for selecting a modelling approach are defined.

In Chapter 6, I reflect upon the achievement of the overall research objective. The comparison of the strengths and weaknesses of the modelling approaches and the analysis of the results and experiences from the research presented in this thesis provides information towards the design of a framework for recommendable practices to model regional patterns of crop yield. The chapter ends with a number of conclusions.

2 Regional crop yield estimates: how to feed our crop growth simulation models?

Crop growth simulation models (CGSMs) are useful tools to estimate crop yield. However, at the regional level, their application is constrained by data requirements. This chapter aims to provide decision rules for selecting appropriate approaches to supply CGSMs at the regional level with suitable weather, soil, and management data. First, we discuss the three main domains of input data by looking at the spatial characteristics of the variable, the availability of data at the regional level, and reviewing the approaches that people have been using to generate input data for CGSM applications at the regional level. Then it uses the review to formulate decision rules as to what approach to take under different circumstances. Which of the approaches should be used depends on the following questions: (i) do observations of the input variable allow to estimate semivariograms?; (ii) are there auxiliary data correlated to the target variable?; (iii) do the input variables exhibit spatial correlation?; and (iv) is there spatial correlation in the residuals of the regression that related auxiliary data to the target variable?. Summarized, the selection of possible approaches depends on the data availability, the spatial variability, the temporal variability, the correlations with other variables, the data acquisition methods, the expected accuracy from a particular approach used to describe spatial variability, and the sensitivity of the CGSM to the variable. This sensitivity makes every decision context specific. At the regional level CGSMs are typically fed by the input data that are generated as discrete zones. However, increasingly the input data are presented as continuous surfaces to feed the CGSMs as a result of the development of new interpolation techniques, the accumulation of data sources (in digital form), and inclusion of auxiliary data. Generally, spatially-explicit regional patterns of yield are less accurate when done for discrete zones compared to continuous surfaces, although one should be aware of a false sense of accuracy, when continuous maps are made by unreliable interpolations. The most suitable method should be selected in a structural way, using decision rules as presented in this chapter, rather than to limit ourselves in an early stage to the typical procedures such as discrete zones.

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2.1 Introduction

There is an increasing call for regional, spatially-explicit yield estimates in the context of e.g. climate change studies and rural development. Crop growth simulation models (CGSMs) are useful tools to provide such estimates under current conditions but also to evaluate the potential effects of environmental, biological, and management changes on crop growth (Hoogenboom, 2000). There is a wide range of CGSMs available, such as the Decision Support System for Agro-technology Transfer (DSSAT; Jones et al., 2003) and the Agricultural Production system SIMulator modelling (APSIM, Thorburn et al., 2010; Keating et al., 2003). Most CGSMs have been designed to simulate crop production for a field, which can be assumed uniform in soil, weather, and management. The models are not specifically developed to assess regional patterns of crop yield. The development of regional models is troubled by the lack of insight in processes specific to the regional level (Veldkamp et al., 2001), but also by the data requirements for their calibration and application. Due to the urgent call from policy makers to assess regional patterns of crop yield, scientists pragmatically use the field-level CGSMs at regional scales (e.g. Tsvetsinskaya et al., 2003; Iglesias et al., 2000; Chipanshi et al., 1999). These studies aim to identify (i) the effect of climate change (e.g. Challinor et al., 2009; Reidsma et al., 2009; Xiong et al., 2008; Wolf and Van Oijen, 2002; Hansen and Jones, 2000), (ii) the impact of changes in land use, policy, and technology (e.g. Godard et al., 2008; Stoorvogel et al., 2004), and / or (iii) annual yield forecasts (e.g. Yun, 2003; Jagtap and Jones, 2002; Chipanshi et al., 1999; Supit and Van der Goot, 1999; Supit, 1997). The target variable of the studies varies as some studies focus on aggregated yield data (e.g. mean and standard deviation) (Faivre et al., 2004; Van Ittersum and Donatelli, 2003; Jagtap and Jones, 2002; Bouman et al., 1996) while others aim at the assessment of regional patterns (Beaujouan et al., 2001; Gomez and Ledoux, 2001; Faivre et al., 2000).

Applying the models at the regional scale has various consequences. Scale is defined on the basis of extent (i.e. the spatial area covered by the simulation), support (i.e. the spatial area covered by the observed data), and resolution (i.e. the ratio between the support and the extent) (e.g. Faivre et al., 2004; Bierkens et al., 2000). As soon as we move towards higher scale levels the extent increases. By increasing the extent of the study, new processes and variables possibly emerge as driving factors behind the variability in crop yield. For example, spatial variability of access to markets can emerge as a determinant of spatial patterns, or a regional variability in sensitivity to plagues and diseases may appear. Thus, with increasing extent it becomes necessary to incorporate additional data (Faivre et al., 2004; Hansen and Jones, 2000). The higher scale level

also means that data on weather, soils, and management are not available at the same resolution. While detailed soil maps may be available at a scale of 1:20,000 for small areas, regional exploratory surveys are typically at a scale of 1:50,000 to 1:250,000. The availability of data on weather, soil, and management is one of the problems that the application of CGSMs at the regional level faces (Carbone et al., 2003; De Bie, 2000; Nachtergaele, 2000; Fresco et al., 1997; Sombroek and Antoine, 1994). Many approaches have been developed to overcome the problem of data availability, but the plethora of available approaches is overwhelming and makes one uncertain about which approaches to use.
CGSMs require input data from three domains; weather, soil, and management. Each of those has very different spatial characteristics. Weather exhibits gradual changes over space, but with a high temporal variability. Weather data are therefore typically collected for a limited number of points in space and with a high temporal resolution. Soil properties are relatively stable over time but with more spatial variability, including abrupt changes. Although soil data are generally collected at the point level, they are often available as soil maps that describe the variability through a limited number of mapping units. Crop management is highly variable, both in space and time. In contrast to soil and weather data, there is little tradition in mapping agricultural management. Therefore, most studies rely on ad-hoc farm surveys. Only in a few cases cross-sectional management data are available.

The purpose of this chapter is to provide decision rules for selecting appropriate approaches to supply CGSMs at the regional level with suitable input data. First, we discuss the three main domains of input data by looking at the characteristics of the variable, available data, and reviewing the approaches that people have been using to feed CGSMs. Secondly, we discuss a number of recent developments in data acquisition that may open new alternatives to provide better estimates of spatial variability of the input data. When regional yield patterns need to be assessed typically the studies do not have the resources to collect new data. We therefore focus on using existing data to estimate the spatial variability of the input data. We use the review to formulate decision rules when to use which approach.
In this study we focus mostly on the spatial element of scale (rather than the temporal element) as we aim to assess spatial patterns of crop yield. We adopt a pragmatic operational definition of the regional level as the scale levels above the field level for which the CGSMs have been developed. As a result, the regional level includes the catchment level but also the national or continental scale levels.

2.2 Assessing spatial variability of growing conditions

Despite the fact that most CGSMs have not been developed for application at the regional scale and that data availability is limited, the literature provides us with a plethora of case studies where CGSMs have been used to assess regional patterns of crop yield. This section reviews the various approaches on the assessment of regional variability in weather, soil and crop management.

2.2.1 Weather variability

Most CGSMs require daily weather data including, for example, precipitation, temperature (minimum and maximum), potential evapotranspiration, and solar radiation. Weather data are characterized by a high temporal variability and generally exhibit gradual changes in space (except for the case of individual rain showers). Data are typically collected for a limited number of weather stations. These stations generally provide data at a high temporal resolution (mostly daily). As a result, we have good insight in the temporal variability, but the information on the spatial variability is limited. The simplest approach to obtain a spatially continuous map of weather data involves a subdivision of a region into discrete zones (Southworth et al., 2000). Weather conditions in each zone are represented by a weather station and the spatial variability within the zone is ignored. Different approaches are used to delineate the weather zones including nearest neighbour, statistical techniques, and expert judgment.

Nearest neighbour interpolation (Thiessen polygons) is the most straightforward methodology. Conceptually the methodology simply uses for each location the data from the nearest weather station. This approach does not use any auxiliary data. Due to its simplicity it is commonly used (Leenhardt et al., 2010; Xiong et al., 2008; Launay and Guérif, 2003; Heinemann et al., 2002; Heywood et al., 1998). Alternatively, weather zones are delineated using statistical techniques in combination with auxiliary data (e.g. Donet et al., 2001; Leenhardt, 1995; Ripert et al., 1990). Auxiliary data which is known to be related to weather, such as altitude, is used to identify zones. In another approach the weather zones are defined by experts and linked to weather stations (e.g. Legros, 1996). Experts draw the weather zone based on their insight, possibly using auxiliary information. The disadvantage of the use of expert judgment is that it is subjective.

Weather data can also be interpolated between weather stations to generate a continuous surface of weather variables. Typical interpolation method is kriging. Most interpolation techniques calculate for each location a weighted average of the observed values at surrounding observation points (in this specific case weather station). They best apply to variables that exhibit continuous spatial variation (e.g. Voltz and Webster, 1990). Interpolation has to be done separately for each weather variable and for each individual time step (e.g. Leenhardt et al., 2006; Hansen and Jones, 2000), which makes the interpolation very time consuming. More commonly, therefore, is that interpolation techniques are applied to temporal averages, such as monthly data. For example, several authors interpolated monthly weather data from weather stations (e.g. Harrison et al., 2000; Saarikko, 2000). It produces good estimates of the spatial variation in monthly weather conditions because of the gradual variations. In some cases the interpolated monthly data are subsequently temporally disaggregated to the daily data required by CGSMs using, for example, a sine curve interpolation method (Brooks, 1943) or stochastic weather generators (Semenov and Barrow, 1997; Racsko et al., 1991; Richardson and Nicks, 1990; Richardson and Wright, 1984).

When auxiliary data are available, other interpolation techniques involving auxiliary data (such as process-based weather models) can be used to interpolate sparse data. The weather models are used to interpolate weather data, using for example digital elevation models (DEMs) (Kumar et al., 2010; Evrendilek, 2007; Baigorria, 2005; Courault et al., 2003; Courault et al., 1998). Baigorria (2005) provides a good example of a process-based interpolation model estimating the spatial and temporal distribution of maximum and minimum temperatures and rainfall in mountainous areas. His model interpolates maximum and minimum temperatures based on the radiation balance at specific hours when those temperatures occur. Rainfall is interpolated based on cloud movements over complex terrains, incorporating the physical processes driving rainfall events. The results are presented as daily maps in which the spatial resolution is controlled by the resolution of the DEM. The development of this kind of process-based approaches is still at a very early stage.

To conclude, regional weather variability is typically described by a limited number of discrete zones. However, increasingly the weather data are presented as continuous surfaces. Despite some of the disadvantages of the use of discrete zones (conceptually weather zones are less accurate compared to continuous surfaces), their use is quite common for weather data. This is probably due to a number of specific properties of weather data. Except for mountainous regions, weather conditions vary gradually resulting in a relatively good description by the weather zones. In addition, weather data are collected at a low spatial resolution that does not allow for more detailed descriptions.

2.2.2 Soil variability

Soil data show, particularly in contrast to weather data, relatively little temporal variability. On the other hand, they present more spatial variability. Traditionally, soil data are acquired through soil surveys in which a large number of field observations is collected (e.g. Soil Survey Staff, 1993). The information of the observations is combined with e.g. additional field observations of topography, aerial photography, and expert knowledge to delineate the mapping units presented on the soil maps. In practice, the spatial perception of soil results in a map in which units are discrete zones with sharply defined boundaries (Burrough and McDonnell, 1998). The mapping units are described by one or more soil types and each of the soil types is represented by a typical soil profile. Soil properties are often derived from a limited number of representative soil profiles described in the soil survey report. Most studies only use the dominant soil type from each mapping unit (Angulo et al., 2012).

Soil types are described by soil profiles for which soil chemical and physical analysis were carried out (e.g. Soil Survey Staff, 1993; Brus et al., 1992; Boulaine, 1980). In many situations, the recorded soil properties are incomplete for the application of CGSMs. A common solution to this problem is the use of pedotransfer functions (PTFs). These are functions that relate basic available soil properties to the more difficult to measure soil properties (Wosten et al., 2001; van Genuchten and Leij, 1992; Bouma, 1989). A good example, in which a variety of PTFs is evaluated, is presented by Gijsman et al. (2003). They evaluated different PTFs to assess soil water retention parameters (e.g. soil water content at field capacity, wilting point and, saturation) as inputs for CGSMs. These are often used at regional scales to quantify required soil properties (e.g. Donet et al., 2001; Leenhardt, 1995). If a large number of soil observations is available, a continuous surface of soil properties can be created by the use of interpolation techniques (see e.g. Soltani et al., 2013).

In soil surveys, point data have been collected to describe soil variability. The original point data have been lost in the process to develop the currently available soil map. Only the representative soil profiles are included in the soil survey reports. As a result, most people use the discrete zones of the soil map. And few cases use interpolation to describe soil variability.

2.2.3 Management variability

Management data required by CGSMs include, amongst other things, the crop varieties, sowing and planting dates, fertilizer management, and irrigation data. Management data are highly variable in space and time. Because of this variability and the lack of proper surveying, data on the spatial variability of management is often unavailable at regional scale (Leenhardt et al., 2010; Godard et al., 2008; Maton et al., 2007; Mignolet et al., 2007; Biarnès et al., 2004; Jagtap and Jones, 2002).

One possible approach is to use typical or recommended practices over the spatial extent (Godard et al., 2008; Yun, 2003; Faivre et al., 2000; Hansen and Jones, 2000). Alternatively, a limited number of discrete management zones can be identified. Experts draw the management zone based on their expertise and survey data (Therond et al., 2010; Janssen et al., 2009; Zander et al., 2009; Godard et al., 2008).
Alternatively, continuous surfaces can be assessed for some variables like sowing dates using remote sensing (e.g. Launay, 2002; Guerif and Duke, 2000). Such surfaces can also be determined using statistical or probability relationships that relate the management practices to other input variables such as rainfall. For example, sowing dates can be calculated based on soil and weather conditions using statistical relationships (e.g. Moen et al., 1994; Leenhardt and Lemaire, 2002).
Another approach to describe the variability in management is by using farm typologies. In a farm typology, farms are grouped on the basis of various characteristics observed in a farm survey. It could be based on cropping patterns but also on resource endowment or farmers' objectives (Mesiti and Vanclay, 2006, 1997; Thomson, 2001a, 2001b; Howden et al., 1998; Vanclay et al., 1998; Vanclay and Lawrence, 1995; van der Ploeg, 1994). Although all farm types can be simulated, most studies only use the dominant or average farm type from each management zone (Salvi et al., 2012). This is comparable to the use of the dominant soil type for soil mapping units.
To conclude, although different approaches exist, most studies use typical farm management to feed the CGSMs. This is probably due to specific properties of management data. Management is highly variable in space and time, and results from human decision-making. Predicting optimal decisions is one thing, and can be inferred from weather, soil and crop data, but predicting actual decisions, which, for a multitude of reasons, deviate from optimal rational decisions, is even much more difficult. Indeed, in comparison to other input data of CGSMs, the availability of management data is limited.

2.2.4 Typical procedure

The use of discrete zones is quite common to describe the variability in weather, soil, and management to assess regional patterns of crop yield. In such a case, individual weather, soil, and management zone maps are overlaid to create a map with zones with unique weather, soil and management conditions. The CGSM can be run for these so-called simulation zones resulting in a map with discrete zones characterized by the resulting simulated crop yield. Figure 2-1 shows this typical procedure. Spatial scales and temporal resolutions of datasets commonly used as input data to feed CGSMs at the regional level are shown in Table 2-1. Weather data are collected for a limited number of points in space and expressed by daily data. Soil data are collected at the point level but in most cases derived from soil maps. Soil properties are relatively stable over time. For management data, we have to rely on ad-hoc farm surveys. Most studies use one set of management data for growing season.

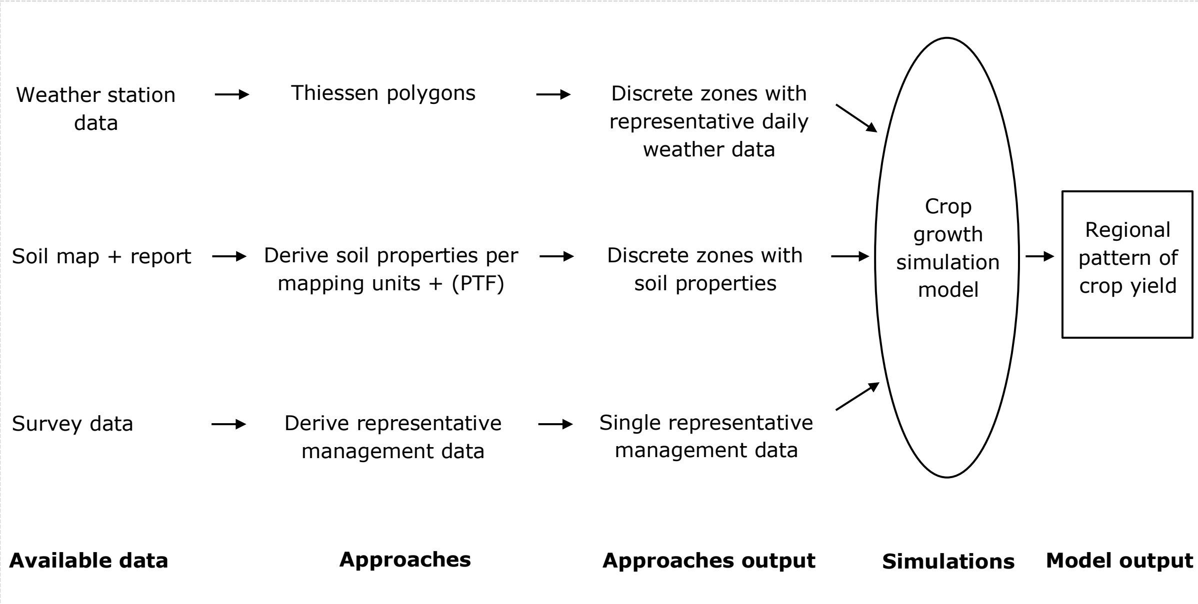


Figure 2-1: Typical procedure to assess regional patterns of crop yield by crop growth simulation models with the use of discrete zones for input data.

Table 2-1: Spatial scale and temporal resolution of datasets used to feed CGSMs at the regional level

Input data		Spatial scale [a]	Temporal resolution	Reference
Weather data	Weather stations	0.1-0.01 km^2	Daily	Soltani et al., 2013; Therond et al., 2010; Bakker et al., 2005; Hansen and Jones, 2000; Southworth et al., 2000.
Soil data	Soil profiles	1- 0.1 km^{-2}	Once	Bakker et al., 2005; Hansen and Jones, 2000.
	Soil units	Units of 1- 5 km	Once	Angulo et al., 2012; Therond et al., 2010; Jones et al., 2000.
Management data	Farm/ field	1-2 km^{-2}	Once	Angulo et al., 2012; Colbach, 2008; Angevin et al., 2002.

[a] expressed as density of observations (for point data) and average size for zone data

2.3 New developments

For quite a while, the use of discrete zones and limited use of auxiliary data is quite common to describe the variability in weather, soil, and management. The discrete zones allow for the assessment of regional patterns of crop yield with a limited number of simulation runs, albeit that the spatial pattern will clearly reflect the soil pattern and the weather and management zones. In the past, limiting the number of simulation runs was an important argument, due to the limited computer capacity. However, with the computer limitations largely resolved, it becomes more interesting to work with continuous surfaces of input data. Availability of auxiliary data and new interpolation techniques increasingly allow for the derivation of continuous surfaces of the input variables.

In this section we review the new developments in obtaining continuous surfaces of weather, soil, and management data. We limit ourselves to the creation of such surfaces from existing data, and do not discuss new acquisition techniques like proximal sensing etc. The opportunities for improving the description of spatial variability differ between the various domains of input data, which is due to the specific properties of each of the input data.

2.3.1 Weather data

The limited number of observation points and the high temporal resolution for weather data limits the application of simple interpolation techniques like kriging. The extent of the study area determines the number of weather stations that are available for a particular study. For example, if the study involves a small catchment (e.g. Soltani et al., 2013) the number of weather stations may be very limited (less than 5). Studies at the national scale may be able to use a relatively large number of weather stations ranging from 100 (for countries like Germany and Ecuador) up to 1200 for the US. The implications are that interpolation techniques like kriging are only possible in studies with a larger extent. The interpolation techniques like regression-kriging may be supported through the use of auxiliary data derived from spatially referenced environmental data layers such as DEMs, such as the global 90-m resolution DEM from the Shuttle Radar Topography Mission (Jarvis et al., 2008). Moreover, remote sensing data can be considered as auxiliary data to use in the interpolation. For example, remotely sensed cloudiness can be used as a proxy for radiation. With sufficient observations the auxiliary data allow for advanced interpolation techniques like regression-kriging. If the number of weather stations is limited and the auxiliary provide a continuous description of the co-variable, a regression is also possible. The regression equation can subsequently be applied to the continuous surface of the auxiliary data to create a continuous surface of the target variable. Weather data itself can also be observed by satellites (e.g. Hansen and Jones, 2000). The big advantage of these measurements is that they directly result in continuous surfaces of weather conditions. Interesting enough there is very little use of mechanistic models to create continuous surfaces of weather data (e.g. Baigorria, 2005) to feed CGSMs.

2.3.2 Soil data

Currently, with improved tools like geographical information systems (GIS) and field computers, more point data are saved during soil surveys than before. Moreover, because soil data do not change much over time, observations typically accumulate over time. The increased availability of soil observations allows for moving from discrete zones to continuous surfaces by means of interpolation. If auxiliary data are available they can also be used to improve the interpolation. An advanced form of interpolation, where the use of auxiliary data is formalized, is digital soil mapping (DSM) (see e.g. Kempen et al., 2011). It applies pedometric methods to map (predict) the spatial variability of soils (Grunwald, 2006; McBratney et al., 2003; McBratney et al., 2000). The conceptual framework of DSM is based on the main soil forming factors: climate, organisms (mainly vegetation), relief, parent material, and time (Jenny, 1941). DSM formalizes the relationships between soil properties and the soil forming factors by deriving empirical relationships between observations on soil properties and auxiliary variables that represent the soil forming factors (McBratney et al., 2003). These auxiliary variables are DEMs, satellite images, and geology maps. Once quantified by a statistical model, the relationships between soil and soil forming factors can be used to predict soil properties at locations where field observations are lacking but auxiliary data are available. Soil spatial variability can be represented with different models of spatial variation. It is generally modelled as a continuous phenomenon with a continuous model of spatial variation (e.g. kriging) but discrete or mixed models of spatial variation can be applied as well (Heuvelink and Huisman, 2000; Heuvelink, 1996). However, DSM has drawbacks of its own. The standard procedures do not provide information on the three-dimensional variability of the soil properties as it is provided by the representative soil profiles for the discrete zones. Recently, few studies have combined general pedological knowledge with interpolation methods to map the three-dimensional variation of soil properties using depth functions (Kempen et al., 2011; Malone et al., 2009; Meersmans et al., 2009; Mishra et al., 2009). Much more research is needed to make these tools applicable for the wide range of soil properties in conjunction with CGSMs.

Direct observation of soil properties by satellites is limited to topsoil, and only for cases where the soil is bare and not too many clouds occur. Finally, there is very little use of improved mechanistic models to create continuous surface of soil properties (e.g. Finke, 2012; Minasny and McBratney, 2001) to feed CGSMs.

2.3.3 Management data

The limited number of observation data and the high variability of management data at short distances limit the application of simple interpolation techniques like kriging. For management practices that depend on individual farmer decisions rather than on physical properties (e.g. fertilizer application), it is often difficult to determine relationships with auxiliary data. Thus advanced interpolation techniques involving auxiliary data are not expected to give good results and this management data can only be derived from farm surveys. Some management data shows reasonable relationships with auxiliary data. For example, Sacks et al. (2010) predicted the global spatial patterns of maize and spring wheat planting dates reasonably well by assuming a fixed temperature at planting. The relationship with temperature can also be useful to create a continuous surface of the planting date. Moreover, continuous surfaces can be assessed for some variables like sowing dates and crop choices using remote sensing (e.g. Launay, 2002; Guerif and Duke, 2000). However, this only results in ex post assessments, and is not useful for future predictions. Much more research is needed to create continuous surface of management data by models (possibly agent-based models) to feed CGSMs.

2.4 Decision rules

Only in exceptional cases, data are collected at the proper resolution for the application of the CGSMs at the regional level. If this is not the case, one will often describe the spatial variability through a subdivision of a region into discrete zones. However, increasingly the CGSM's input data take the form of continuous surfaces, which allow for better crop yield estimates. This development is due to the development of new interpolation techniques, the accumulation of data sources (in digital form), and inclusion of auxiliary data. This review shows that there is a wide array of methodologies available, although criteria for the selection of the methods are often unclear. Which of these should be used depends on a number of questions whose answers lead to the decision rules denoted in Figure 2-2. These criteria followed largely from literature review and are discussed in the following.

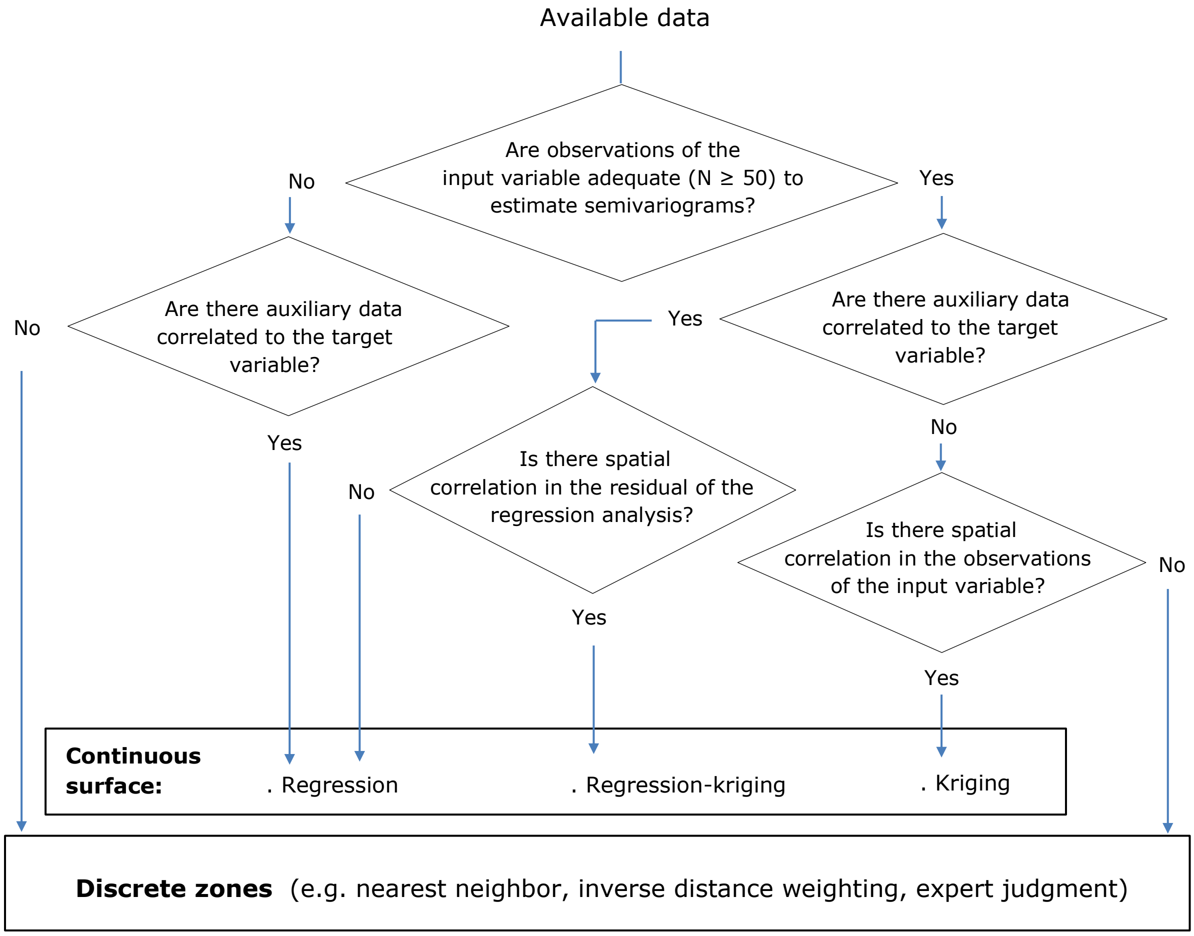


Figure 2-2: Decision rules for selecting appropriate approaches to describe the spatial variability of input variables to feed crop growth simulation models at the regional level (scale effects not included).

(i) Are observations of the input variable adequate to estimate semivariograms?

The approaches to create continuous surface variables are referred to as "geostatistics" (Goovaerts, 1997; Journal and Huijbregts, 1978). Geostatistical methods can be considered interpolation techniques. To apply geostatistics, a "semivariogram" must be estimated (see Figure 2-3), which shows the magnitude of spatial variation as a function of distance (Goovaerts, 1997). The semivariograms can only be estimated if the number of observations of the variable is large enough (Webster and Oliver, 1992) and has an acceptable point density. In general, at least 50 observations are required, of which at least some pairs are at close distances in order to correctly estimate the nugget (e.g. Tabachnick and Fidell, 1996; Comrey and Lee, 1992). If this is not the case, other interpolation techniques such as nearest neighbour and inverse distance weighting that do not use the semivariograms can be used to generate input data as discrete zones.

The advantage of geostatistical methods over nearest neighbour and inverse distance weighting interpolation is that a measure of accuracy of the estimate is provided. The difference between them is that with nearest neighbour and inverse distance weighting interpolation the weights assigned to sample data depend solely on the sample configuration, whereas with geostatistics methods the weights depend on both the sample configuration and a model of spatial variation estimated from the data (i.e. semivariogram).

(ii) Is there spatial correlation in the observations of the input variable?

Once the semivariogram is made, one can determine the spatial correlation in the data. The idea underlying all the interpolation methods is that spatial autocorrelation between two observations declines with the distance between these observations. Therefore, variance increases with increasing distance, until the overall variance of the variable is achieved, termed the ''sill'', which happens at a distance termed the ''range''. The range represents the distance beyond which there is no spatial autocorrelation. For very small distances the variance, termed the ''nugget'', although a minimum, may still be non-zero; it can be caused by a discontinuous surface or by measurement error (Goovaerts, 1997). Figure 2-3 shows a schematic semivariogram, adapted from Eleveld and van der Woerd (2006). The "nugget-to-sill" ratio and the "range-to-extent" ratio can be used to explain (classify) the spatial correlation. The lower "nugget-to-sill" ratio for observed data indicates a stronger spatial correlation of the input variable. For instance, Cambardella et al. (1994) classified spatial correlation of soil properties by using the "nugget-to-sill" ratio as follows: a ratio more than 75% indicates a weak spatial correlation; a ratio less than 25% indicates a strong spatial correlation; and a ratio between 25% and 75% indicates a moderate spatial correlation. The larger "range-to-extent" ratio for observed data indicates a stronger spatial correlation of the input variable. When the variable exhibits spatial correlation, the resultant semivariogram can be used to interpolate and predict values in unobserved regions. In doing so, all unknown observations that lie within the range of known observations, are estimated using the information of the known observations. More details regarding the methods that use the semivariogram can be found in Atkinson and Lewis (2000) and Isaaks and Srivastava (1989).

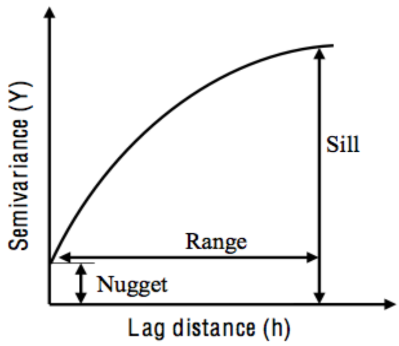


Figure 2-3: A schematic representation of a semivariogram, adapted from Eleveld and van der Woerd (2006).

(iii) Are auxiliary data correlated to the target variable?

In the last decades there has been a surge of auxiliary data including satellite images and DEMs. If the auxiliary data is ratio or interval, geostatistical methods involving auxiliary data e.g. Regression-kriging (Bourrenane et al., 1996) and regression (e.g. Brus, 2000) may be used to create continuous surface of variables. If the auxiliary data is nominal, it can be still used for defining discrete zones (Dobson, 1990). The use of auxiliary data will be more successful when its coverage is higher (it should have a higher coverage than the variable to be described spatially), and when it is more closely related to the input data of CGSMs (the auxiliary data should explain some of the variance of the input data of CGSMs). Last but not least, the ability of the researcher for identification of potential co-variables as such is to be mentioned (process-knowledge) (Bierkens et al., 2000). For more extensive reading about the use of auxiliary data, see Brus (2000), Brus and De Gruijter (1997), and Goovaerts (1997).

(iv) Is there spatial autocorrelation in the residuals of the regression analysis that relates the auxiliary data to the target variable?

The relationship between the observations of the input variable and the related auxiliary data is quantified using regression analyses. Afterwards, the residuals are defined as the real observed input variable minus the value predicted by regression. The spatial correlation in the residuals of the regression can be characterized by a semivariogram. The "nugget-to-sill" ratio and the "range-to-extent" ratio can be used to explain (classify) the spatial correlation as described in section (ii). In the case of spatial correlation in the residuals from the regression analysis, this suggests that omitted explanatory factors exhibit spatial autocorrelation. In such a case geostatistical methods such as regression-kriging can be applied so as to mimic this omitted explanatory factor. In practice, the residuals from the regression analysis are interpolated with kriging, after which the final predicted value is obtained by summing the value predicted by regression and the interpolated residuals (Odeh et al., 1995).

When there is no spatial correlation in the residuals from the regression analysis, a regression suffices to describe spatial variation of the input data. For example, if the number of weather stations is limited, but an auxiliary variable provides a continuous description of the surface in between the observations of the target variable, a regression is a good method to obtain the values in between these observations. That is, the regression equation is applied to the continuous surface of the auxiliary data to create a continuous surface of the target variable.

2.5 Discussion and conclusion

Decision rules concerning appropriate approaches to describe the spatial variability of variables to feed CGSMs at the regional level are presented in Figure 2-2. To structure the review of approaches that have been used in the literature we distinguished between two categories: (i) where input data are generated as discrete zones; and (ii) where input data are generated as continuous surfaces. In the case of discrete zones the CGSM simulations are done for individual discrete zones. In the case of continuous surfaces the CGSM simulations are done for individual grid cells. Obviously, the latter approach is more sophisticated, and likely to result in more accurate spatially-explicit yield predictions. However, in order to generate continuous surfaces, a few conditions need to be met, which are outlined in the decision tree in Figure 2-2. Furthermore, creating continuous surfaces requires more effort, time, and information. The effort may not be worth it if (i) the results are deemed to be just as inaccurate as the discrete zones, or (ii) the CGSM is hardly sensitive to the input variable. Below, we discuss these two aspects, which should contribute to the information based on which the best approach for creating the required CGSM input data is selected.

(i) The accuracy of the presentation of the spatial variability of input data by various approaches is influenced by the accuracy of the original available data, density and spatial pattern of the original available data, characteristics of the study area, and the expected accuracy from a particular approach used to describe spatial variability of input data. The resulting accuracy in the spatial variability of input data generated by various approaches is specific to each case study and difficult to generalize. For example, continuous surfaces often create a false sense of accuracy, which is less so for discrete zones: with these everyone sees that these are simplifications. With continuous surfaces that are derived from shaky data with weak (auto)correlations, one does not see that the results make probably little sense. It is the user's responsibility, then, to prevent introducing the false sense of accuracy and precision unwarranted by the available data. Therefore, if we are able to delineate proper zones on the basis of auxiliary data, this may be preferred above an interpolation to create a continuous surface with a limited number of observations.

(ii) The sensitivity of the CGSM outcomes to a particular input variable is an important factor in determining how much effort one wants to spend on generating an accurate surface. A sensitivity analysis can help to distinguish important from less important variables driving crop yield at the regional level. The approach to create a surface of a variable can be adapted to the sensitivity of the model to that particular variable. Few studies have explored the required level of detail for weather and soil characteristics (e.g. Olesen et al., 2000; Easterling et al., 1998). This is specific to each case study and difficult to generalize.

To conclude, the selection of possible approaches depends on the data availability, the spatial variability, the temporal variability, the correlations with other variables, the data acquisition methods, the expected accuracy from a particular approach used to describe spatial variability, and the sensitivity of the CGSM to the variable. This sensitivity makes every decision context specific. At the regional level CGSMs are typically fed by the input data that are generated as discrete zones. However, increasingly the input data are presented as continuous surfaces. This has the following reasons: (i) the surge of available auxiliary data including satellite images and DEMs; (ii) the accumulation of data sources (in digital form); and (iii) the development of interpolation techniques such as DSM that effectively uses auxiliary data. Generally, spatially-explicit regional patterns of yield are less accurate when done for discrete zones compared to continuous surfaces, although one should be aware of a false sense of accuracy, when continuous maps are made by unreliable interpolations. The most suitable method should be selected in a structural way, using decision rules as presented in this chapter, rather than to limit ourselves in an early stage to the typical procedures such as discrete zones.

3 How to use field-level crop growth simulation models to simulate regional patterns of crop yield?

There is an increasing demand for spatially explicit predictions of crop yield at the regional scale. Two different approaches exist to generate regional patterns of crop yield using crop growth simulation models (CGSMs): (i) run the CGSM for a series of points distributed throughout a region after which the simulated crop productions can be interpolated to create a continuous surface of crop yield (calculate first, interpolate later; CI), and (ii) create surfaces for each of the input variables individually, then run the CGSM for each location (grid cell) to create a continuous surface of crop yield (interpolate first, calculate later; IC). We evaluate and compare these two approaches, by applying a CGSM for potato to two watersheds in the Carchi province in Northern Ecuador. We examine scaling effects that arise from spatial variability in soil properties by using different supports. Model performance was compared with interpolated, observed yields at resolutions of 100 m and 400 m. Results demonstrate that the order of calculation and interpolation was of major importance, while aggregation had a minor effect on the regional patterns of potato yield. The former is probability due to the non-linearity of CGSM and the difference in the spatial dependency of individual inputs. The latter is probably due to the absence of local extremes, which is due to the gradual trends in soil properties in the volcanic ash soils of Carchi (being a result of the soil forming processes, but also a consequence of the interpolation method, kriging). The RMSD in the normalized yields was 0.79 for the CI approach and 0.99 for the IC approach at 100 m. For the aggregation to 400 m, the RMSD was 0.74 for the CI approach and 0.99 for the IC approach. The spatial comparison of regional patterns of crop yield shows that regional yield patterns generated by different procedures (i.e. different approaches and different supports) were similar, while, non-spatial comparisons of different yield patters in terms of RMSD showed better performance of the CI approach than the IC approach. From an uncertainty propagation and variability point of view it is in general preferable to calculate first before interpolation.

Based on: Soltani, A., Bakker, M.M., Stoorvogel, J.J. and Veldkamp, A. How to use field-level crop growth simulation models to simulate regional patterns of crop yield? To be submitted to Agroforestry Systems.

3.1 Introduction

The demand for spatially-explicit predictions of regional crop-yield patterns is increasing. Policymakers need these predictions for e.g. regional development plans, the assessment of climate change impacts, and the reduce the threat of regional imbalances between food supply and demand (Lobell and Ortiz-Monasterio, 2007; De Wit et al., 2005; Jagtap and Jones, 2002). The support level at which model outputs generally become interesting for policymakers is at the level larger than the field support. Agricultural census, other forms of direct surveys, or remote sensing imagery (Khan et al., 2010; Launay and Guerif, 2005) allow to assess spatial patterns of crop yield, but this will only provide insight ex post. An alternative approach to assess a priori and/or future ranges of alternative scenarios spatial yield patterns at the regional scale is the application of modelling approaches such as crop growth simulation models (CGSMs). Since, no process-based CGSMs have been specifically developed to estimate spatial patterns of crop yield at the regional level, field-level CGSMs are frequently being used to estimate the regional patterns of crop yields (e.g. Launary, 2002; Gomez and Ledoux, 2001; Faivre et al., 2000).

The most commonly applied methodology is to run a CGSM for a series of points distributed throughout a region after which the simulated crop yields can be interpolated to create a continuous surface representing the spatial patterns of crop yield (Leterme et al., 2007; Sinowski et al., 1997; Bosma et al., 1994). This methodology, referred to as 'calculate first, interpolate later', is very appealing as the CGSM is applied at the spatial scale for which it has been developed. However, this approach requires high quality weather, soil, and management data to be collected at the same point locations. As this is generally not the case, required data need to be estimated from surrounding observations.

Alternatively, we can create continuous surfaces for each of the variables individually. The CGSM can then be run for each location (grid cell) to create a continuous surface representing the spatial patterns of crop yield (Van Bodegom et al., 2002; Heuvelink and Pebesma, 1999; Bosma et al., 1994). This approach is referred to as 'interpolate first, calculate later'. The advantage is that the procedures followed for the different variables can be specifically designed for the available data. At the same time the procedures can be adapted to the sensitivity of the model to that particular variable.

So far, the two approaches, i.e. 'calculate first, interpolate later' (CI) and 'interpolate first, calculate later' (IC), have been applied in various studies (Leterme et al., 2007; Tong et al., 2007; Van Bodegom et al., 2002; Bosma et al., 1994; Addiscott and Bailey, 1990). The results demonstrate considerable discrepancies. In theory the two approaches are expected to produce the same result when the CGSM is linear, and the interpolation method is linear (e.g. Heuvelink and Pebesma, 1999). When the model and/or interpolation method are nonlinear, the IC and CI approaches produce different results (Groot et al., 1998; Heuvelink, 1998; Addiscott and Tuck, 1996; Addiscott, 1993). It can be quite difficult to anticipate how this non-linearity will exactly affect the differences between the two approaches, but one can expect the deviation to be proportional to the degree of non-linearity of the model or interpolation method (Addiscott and Tuck, 2001).

Hence, an empirical comparison of the two approaches is needed to determine the most suitable approach experimentally, for a specific situation. Although such a comparison has been done before (e.g. Bosma et al., 1994), this was only in a statistical sense (i.e. the root mean square difference) without considering the spatial pattern. Moreover, to our best knowledge, none of previous studies accounted for the effect of the model calculations and interpolations sequence at supports larger than the field support. Spatial aggregation of field support is needed to obtain the regional pattern predictions, and is likely to further exacerbate the differences between the IC and CI approaches.

We studied the effect of the CI and IC approaches on spatial crop-yield patterns at different supports. The SUBSTOR-potato model (Ritchie et al., 1995) was used to model the spatial pattern of potato yield in the Carchi province in Northern Ecuador. The Carchi province was chosen as a study area because the SUBSTOR-potato model (Ritchie et al., 1995) was calibrated and validated in this area. The study focused particularly on the soil conditions for which a relatively large dataset was available.

The specific objective was (i) to find the influence of the sequence of model calculations and interpolations (i.e. CI and IC) on the prediction of spatial patterns of potato yield in the Carchi province at the regional scale, and (ii) to evaluate the persistence of the CI and IC results with different supports, both spatially and non-spatially. Scaling effects of different supports were examined by interpolation of either input or output at a spatial resolution of 100 m and then aggregate them to 400 m. The model performance was compared with interpolated, observed yields at 100 m and 400 m supports.

3.2 Materials and methods

3.2.1 Study area

The agricultural system in the Carchi province, largely situated in the Andes, is dominated by the production of potatoes and milk. The research focused on an area of approximately 36 km^2, comprising two watersheds, ranging in altitude between 2750 and 3450 m above sea level, located at 77°50' Western longitude and 00°37' Northern latitude (Figure 3-1). Being close to the equator there is virtually no change in average monthly temperature, which ranges between 9 and 12°C. However, daily temperatures can vary by more than 10°C. This large swing is caused by the complex mountainous topography, even allowing for severe frost during clear skies at night. Average rainfall varies between 950 and 1300 mm yr^{-1}, and increases with elevation. Volcanic ash soils with their typical thick (about 120 cm), black A-horizon have developed in relatively young volcanic ash deposits. The soils are rich in organic matter (5-14 %) content and have a high infiltration capacity. Generally, at higher elevations (above 3000 m.a.s.l.) younger ash deposits are predominant. The geographic position and climatic conditions allow for continuous plant growth, making the province a very productive agricultural region. The potato farming system in Carchi is intensive and commercial with yields of up to 21 t ha^{-1} as a result of agro-ecological conditions in combination with the access to national and international markets (Crissman et al., 1998). The intensive and continuous production farming does not only result in high productivity but also in a high pest- and disease-pressure, resulting in high rates of pesticide use. Farming in Carchi evolved towards a market-oriented potato-pasture system based on a three to five year rotational system. Farmers follow this rotation with one or two years of "rest" in spontaneously occurring grassland for dairy and meat cattle (Crissman et al., 1998). Due to the intensive form of agriculture, the system strongly depends on external inputs to maintain soil fertility and control pests. Essentially, all potato growers in Carchi used chemical fertilizers, with an average application rate being 138 kg ha^{-1} of Nitrogen, 327 kg ha^{-1} Phosphorus, and 163 kg ha^{-1} Potassium. In addition, farmers apply high rates of Carbofuran, a highly toxic pesticide (Crissman et al., 1998). Intensive input use reduced the gap between potential, nutrient limited yield and the actual yield. Hence, potato growth in Carchi can be usefully modelled by CGSMs.

3.2.2 Data

This study makes use of a 2-year dynamic survey including 40 farms with a total of 187 agricultural fields with 202 observations of potato yields (Figure 3-1; Crissman et al., 1998). The survey includes the detailed registration of crop yields and agricultural management such as planting date and fertilizer applications. Different potato varieties are grown in the study area. To overcome this variability in potato varieties, the yield data are expressed as quality adjusted potato yield based on the relative price levels of the different potato varieties (Crissman et al., 1998). Weather data, including rainfall, maximum and minimum temperature, and solar radiation were recorded daily at the weather stations of San Gabriel, El Angel, and El Voladero around the study area (Figure

3-1). A digital elevation model (DEM), based on 1:50,000 topographic maps, was available for the area (50 m grid size, 2.5 m vertical resolution). For soil properties, a database of 256 soil profiles with full profile descriptions (Meyles and Kooistra, 1997) was used. Table 3-1 provides an overview of the data used as input for the CGSM.

3.2.3 The crop growth simulation model

In this study we used the SUBSTOR-potato model (Ritchie et al., 1995) to obtain spatially explicit predictions of potato yields at the regional scale, as a function of environmental factors. SUBSTOR is a CGSM that simulates the physical, chemical, and biological processes in the potato plant. SUBSTOR is available within the Decision Support System for Agro-technology Transfer (DSSAT) (Jones et al., 1998). The details of SUBSTOR are described by Griffin et al. (1993) and Ritchie et al. (1995). Bowen et al. (1999) and Clavijo (1999) calibrated and validated SUBSTOR for Andean conditions using experimental data from the Carchi area. The weather, soil, and management data considered in the application of SUBSTOR are listed in Table 3-1. Farm management data from the survey showed a large variability in terms of planting date and fertilization (Crissman et al., 1998), but did not show a clear spatial autocorrelation. Therefore, it was decided to use representative management data with a nitrogen application of 168 kg ha^{-1} $season^{-1}$ planted on February 15 for this study.

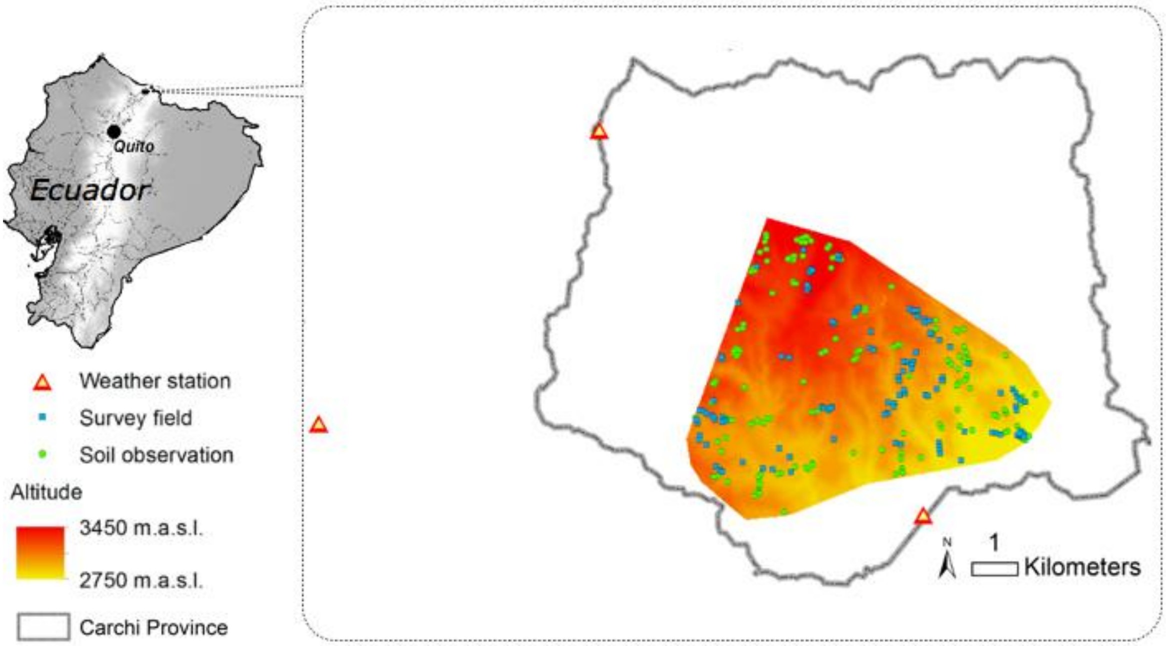


Figure 3-1: Overview of the Carchi study area in Northern Ecuador showing altitude, survey fields, soil observations, and weather stations.

Table 3-1: Total set of variables, with average values for weather, soil, and potato management in the Carchi study area, used by the CGSM.

Weather		Soil (0-50 cm)			Management	
Rainfall (mm/day)		SLOC	Soil organic carbon (%)	4.7	Planting date	Feb 15
Average annual	3.24	SLCL	Clay (%)	28	Fertilizer (kg N h^{-1} season $^{-1}$)	168
Growing season	3.95	SLLL	Water content at wilting point (cm^3 cm^{-3})	0.30	Harvest date	August 15
Maximum Temperature (˚C)		SDUL	Water content at field capacity (cm^3 cm^{-3})	0.46		
Average annual	14.3	SSAT	Water content at saturation (cm^3 cm^{-3})	0.50		
Growing season	15.0	SBDM	Bulk density (cm h^{-1})	1.03		
Minimum Temperature (˚C)		SLNI	Total Nitrogen (%)	0.4		
Average annual	4.6	SSKS	Saturated hydraulic conductivity (cm h^{-1})	0.1		
Growing season	4.6	SCEC	Cation exchange capacity	25		
Solar radiation (MJ m^{-2} d^{-1})		SLHW	pH in water	5.4		
Average annual	13.2	SLHB	pH in buffer	4.5		
Growing season	13.0	SLSI	Silt (%)	31		

3.2.4 Calculate first, interpolate later

For the CI approach, potato yields were simulated for the original 256 soil profiles using the CGSM (Figure 3-2). Since weather data was only recorded at the three weather stations, weather data was interpolated to a 100 m grid between the three meteorological stations using the DEM assuming a linear relationship with altitude. The 100 m grid cells roughly correspond to field size. Subsequently, potato yields were simulated using the observed soil properties, interpolated weather data, and representative management data. Finally, the simulated yields were interpolated using ordinary kriging. Ordinary kriging is often used for spatial interpolation of point data as an optimal interpolator in ecological studies (e.g. Voltz et al., 1990). Hereto, the semivariogram of yield data had to be determined, which characterizes the spatial autocorrelation of the data (Goovaerts, 1997). More details can be found in Isaaks and Srivastava (1989) and Atkinson and Lewis (2000). The quality of the interpolation was evaluated by a cross validation in which the Root Mean Squared Different normalized to the mean of the observed values (CV-RMSD) was used and calculated as:

$$CV - RMSD = \frac{\sqrt{\sum_{i=1}^{n}(\hat{x}_i - x_i)^2/n}}{\bar{x}} \tag{3.1}$$

Where x_i is the simulated yield, $\hat{x}_i$ is the interpolated, simulated yield at location *i*, $\bar{x}$ is the average simulated yield, and *n* is the number of observations. The cross validation involved consecutively removing a data point, interpolating the value from the remaining observations and comparing the interpolated value with the simulated point value (Mueller et al., 2004). Finally, the patterns that were generated were aggregated to a larger support of 400 m to explore the effect of aggregation on the IC and CI approaches.

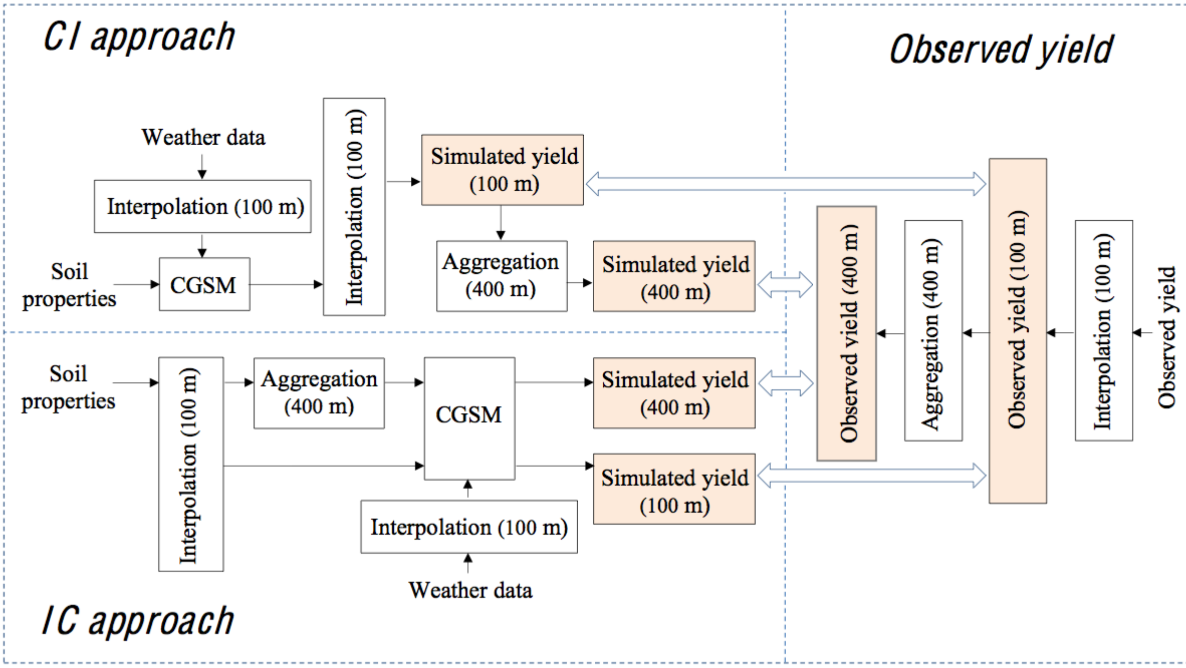


Figure 3-2: Overview of the procedures to evaluate the regional patterns of potato yields in the Carchi study area in Northern Ecuador.

3.2.5 Interpolate first, calculate later

For the IC approach, not only the weather data but also the individual soil properties were interpolated to generate a continuous surface of the necessary input for the CGSM (Figure 3-2). The weighted average of the soil properties over the top 50 cm was calculated and interpolated using ordinary kriging to a 100 m resolution grid. The semivariogram of soil properties had to be determined before interpolation. Then, the quality of all the interpolated soil properties at a 100 m grid was evaluated by a cross validation similar to Eq. (3.1). Only the top 50 cm of the soil profile, i.e. the rooting depth, was considered as this was found to be driving the potato production in a sensitivity analysis. In the sensitivity analysis, soil depth was altered by increasing or decreasing its value by its standard deviation from its mean while holding the other model input variables constant (see e.g. White et al., 2000; Box et al., 1978). After each change in soil depth, the CGSM was run and the simulated response in crop yield was evaluated.

Returning to the IC approach, the CGSM was run for all the individual grid cells. Next, the grids with soil properties were aggregated to 400 m grids to evaluate the performance of the CGSM at a larger support. Also here, the CGSM was run for all the individual grid cells.

In general, with interpolation and / or aggregation variability of data will decrease and local extremes will be levelled out (Baron et al., 2005; Bodegom et al., 2002; Bouma et al., 1996). Depending on the spatial distribution, this effect will be stronger for some variables than for others. As a result, correlations between variables may change with interpolation and / or aggregation. Such changes will have implications for model outcomes and may also be a cause of difference between the results of the CI and IC approaches (Van Bodegom et al., 2002; Heuvelink and Pebesma, 1999). Therefore, three Pearson correlation matrices were calculated to indicate the degree of colinearity between all soil properties at point level, at 100 m, and at 400 m resolutions.

3.2.6 Inter-comparison of the results

The various analyses provided us with four maps describing the patterns in potato yields with differences in approaches (CI and IC) and supports (100 m and 400 m). In order to evaluate the outcomes, a comparison with observed yields was done. Therefore, the observed yields were also interpolated using ordinary kriging. Yield data typically present a significant variability at short distances due to management differences (on top of the agro-ecological differences that are also considered in the CGSMs). Therefore, we paid specific attention to the semivariogram before interpolating to evaluate the spatial dependency. The quality of the interpolated, observed yield at a 100 m grid was evaluated by a cross validation similar to Eq. (3.1). To compare patterns at the appropriate support the interpolated, observed yields were also aggregated to a 400 m grid. Due to the wide range of potato varieties, the yield maps based on the actual observations are expressed in quality adjusted potato yields. However, the simulated potato yields are expressed in nutrient and water limited yields. Given the fact that we are interested in patterns in the potato yield and to make the maps inter-comparable, all six maps were normalized as $(\hat{Y}-\bar{Y})/Y_{sd}$ with $\hat{Y}$ the estimated yield (either observed or modelled yield), $\bar{Y}$ the average yield over the entire map, and Y_{sd} the standard deviation of the yield for the map. The maps are compared in terms of the Root Mean Squared Difference (RMSD). The RMSD is calculated as:

$$RMSD = \sqrt{\frac{\sum_{i=1}^{n}(\hat{x}_i - x_i)^2}{n}} \qquad (3.2)$$

where x_i is the interpolated, observed yield, $\hat{x}_i$ the model-based yield for cell *i*, and *n* is the number of cells. To compare visually the simulation maps of the CI and IC with the interpolated, observed yield, the simulated maps from the two approaches were grid-by-grid subtracted from the observed-interpolated yield map at each resolution to reveal the differences (over- or underestimations) in predicted values. Moreover, spatial dependency of the CI and IC results were assessed in terms of semivariogram parameters (i.e. nugget-to-sill ratio and range) and Moran's I (Li et al., 2007; Moran, 1950). Moran's I values range from −1 (indicating perfect dispersion) to +1 (perfect dependency). A zero value indicates a random spatial pattern. Hereto, the grids of the CI and IC maps were converted to point data and then the semivariogram and Moran's I were applied to the point data using ArcMap 9.3.

3.3 Results and discussions

3.3.1 Non-spatial comparison of simulated yields and observed yields

The CI approach vs. IC approach

In the Carchi study area, the CI maps presented smaller RMSD values than the IC maps. The RMSD of the normalized yields was 0.79 for the CI approach, 0.99 for the IC approach at 100 m. It is assumed that non-linearity of the model plays a key role in difference between the results of the CI and IC approaches. Moreover, there are other factors including the spatial dependency of soil properties, and the correlations between the soil properties that may play a role in difference between the results of the CI and IC approach (see e.g. Van Bodegom et al., 2002; Addiscott and Tuck, 2001; Heuvelink and Pebesma, 1999). Anticipating how these factors' interactions will affect the differences between the two approaches is difficult. Therefore, in this study I took an experimental approach to understand and consider the role of these different factors in the differences between the two approaches.

In the Carchi region, all soil properties were characterized by a nugget-to-sill ratio less than 41%, a range of about 3.5 km, and a CV-RMSD of 8 - 10 %. The large range (compared to the size of the study area) was expected in the Carchi study area as most soil properties vary gradually with climatic differences and with various ash deposits (Crissman et al., 1998). The individual inputs (i.e. soil properties in this case) showed different spatial dependency. Although these differences were small, they can explain the difference between the results of the CI and IC approach. This is because interpolation of the individual inputs can take these differences into account whereas spatial interpolation of the output cannot (see e.g. Heuvelink and Pebesma, 1999). On the other hand, the output of the CGSM had an even larger range (>3.5 km, with a nugget-to-sill ratio of 38%, and a CV-RMSD of 11%) than the ranges of soil properties. This may be due to the general trend in weather variables and also effect of the nonlinear model. Interaction of model non-linearity with the spatial dependency of inputs increases the range in the CI approach (Leterme et al., 2007).

A Pearson correlation matrix was calculated to indicate the degree of colinearity between all soil properties at point level (Table 3-2). The matrix shows that some of soil properties are strongly correlated. Since correlations between variables may change with interpolation, this is a potential cause for differences between the CI and IC approaches. Therefore, a Pearson correlation matrix was also calculated to indicate the degree of colinearity between all soil properties at 100 m resolution (the same result as Table 3-2 was obtained). However, in this case study, the data correlation between all soil properties did not change from point level to 100 m resolution. It is therefore concluded that in this case study the difference between the results of the CI and IC approaches was caused by the non-linearity of the model and the differences in the spatial dependency of various soil properties.

Although smaller values of RMSD mean that the CI approach performed better than the IC approach, the IC approach should not automatically be discarded. Especially when the CGSM requires high-quality weather, soil, and management data that are not collected for the same point locations, and available data still need to be estimated from surrounding observation points. For example, in this case study, weather data was only recorded at the three weather stations, and the only possible option was to interpolate weather data between the three meteorological stations. To generate reliable model results for regional application and/or estimate associated uncertainties, it is important to understand and consider the effects of such data interpolation on simulation results.

Table 3-2: Pearson correlation coefficients between soil properties in the crop growth simulation model

	SBDM	SCEC	SDUL	SLCL	SLHB	SLHW	SLLL	SLNI	SLOC	SLSI	SSKS	SSAT
SBDM	1											
SCEC	-0.44	1										
SDUL	-0.45	0.86	1									
SLCL	0.19	-0.08	-0.35	1								
SLHB	0.77	-0.47	-0.63	0.49	1							
SLHW	0.79	-0.52	-0.66	0.62	0.88	1						
SLLL	-0.47	0.85	1	-0.36	-0.64	-0.66	1					
SLNI	0.06	0.33	0.52	-0.58	-0.31	-0.42	0.53	1				
SLOC	0.15	0.35	0.51	-0.51	-0.20	-0.33	0.51	0.96	1			
SLSI	0.41	0.08	0.04	0.21	0.34	0.26	0.02	0.40	0.49	1		
SSKS	0.68	-0.84	-0.89	0.32	0.73	0.78	-0.88	-0.42	-0.38	0.03	1	
SSAT	0.41	0.13	-0.07	0.38	0.70	0.56	-0.10	-0.22	-0.11	0.24	0.23	1

For acronyms of soil properties, see Table 3-1.

The CI and IC approaches at different supports (aggregation)

For the CI approach, the agreement between simulated and observed yield slightly increased with increasing support (aggregation of the model output). The RMSD in the normalized yields was 0.79 at 100 m and 0.74 at 400 m. This was expected as the variability decreases with aggregation and local extremes are levelled out (Baron et al., 2005; Hansen and Ines, 2005; Easterling et al., 1998). This was also found by Verburg et al. (1999) and Kok and Veldkamp (2000). In their model validation they found that deviations between modelled and actual land use at the cell level can be considerable, but that very good agreement was found at higher aggregation levels such as agro-ecological zone or district. The results showed that aggregation of calculated data leads to less variability and increasing linear fits at higher aggregation levels. The spatial variability in the case study area determines how strong this effect is.

For the IC approach, the agreement between observations and simulation remained constant with spatial aggregation. The RMSD in the normalized yields was 0.99 at both supports (i.e. 100 m and 400 m). This is because the aggregation effect on the soil properties was quite small in the study area (aggregation of the model input). Data on soil properties were obtained from interpolation of 256 soil profiles, and because of this interpolation, local extremes did not exist, not even at fine resolutions. For that reason, aggregation did not have a very strong effect. Moreover, from Table 3-2, it can be seen that some of soil properties are strongly correlated. When correlated variables are multiplied or divided in a model, aggregation can lead to severe scaling errors. Therefore, a Pearson correlation matrix was also calculated to indicate the degree of colinearity between all soil properties at 400 m resolution (the same result as Table 3-2 was obtained). However, in this case study, the data correlation between all soil properties did not change from point level to 400 m resolution. For that reason, aggregation did not have a very strong effect. Moreover, the soil properties are probably not subject to local extremes (meaning that it is not only a consequence of the data interpolation). Because of the gradual trend of the young and older volcanic ash soils in the region, adjacent locations tend to be more similar, and hence the change in variability with aggregation becomes less (see e.g. Reynolds and Amrhein, 1998). Therefore, it was expected that the aggregation of soil properties has a relatively small effects on the prediction of potato yield. Moreover, it has to be taken into account that this study covers a region in which high input agriculture. As the provision of nutrients is one of the main functions of the soil, it is not surprising that the aggregation of soil data results in only minimum levelling-out of extreme values. The result was in line with conclusions from other studies (Folberth et al., 2012; De Wit et al., 2005; Olesen et al., 2000; Easterling et al., 1998).

In this study, aggregation had a minor effect on the prediction of the spatial pattern of potato yield because of the gradual trend in soil properties. However, at the regional level, soil properties generally exhibit more (short-distance) spatial variability. Moreover, no process-based CGSMs have been specifically developed to estimate regional patterns of crop yield. The application of field-level CGSMs at supports larger than fields may require an adaptation of the model (re-calibration) because relations between variables that exist at the field support need not extend to the larger support. Another alternative procedure to avoid application of the field-level model at a larger support is to use the route in which the model is run at field support (i.e. the 100 m grid cells roughly correspond to field size), and then to aggregate the model output (see e.g. Heuvelink and Pebesma, 1999). Therefore, in the case that available data still need to be interpolated from surrounding observation points (i.e. IC), the aggregation step can be applied after model calculation in the sequence because of model non-linearity. For example, Soltani et al. (2013) aggregated the all yield maps (observed and the IC approach-based) to larger spatial aggregations levels to estimate regional patterns of crop yield at supports larger than field. They concluded that increasing the level of spatial aggregation increased the similarity between simulated yield patterns and interpolated, observed yield. Similar results have been found by Leterme et al. (2007).

3.3.2 Spatial comparison of simulated yields and observed yields

The spatial variability of the observed yield was characterized by a nugget-to-sill ratio of 58%, and a correlation range of 3 km. The semivariogram of the observed yields indicates a moderate spatial autocorrelation. The 202 yield observations were interpolated with ordinary kriging. The cross validation revealed a CV-RMSD of 17%. The resulting map demonstrated that the higher yield levels are attained in the western part, where altitudes are between 3000 and 3300 m.a.s.l. The results demonstrate a yield decrease towards warmer and dryer conditions, which coincide with lower elevations. The maps of the different approaches at different supports showed a similar spatial pattern (results are not shown). To compare visually, the simulated maps from the two approaches were grid-by-grid subtracted from the observed-interpolated yield map at each resolution to reveal the differences (over- or underestimations) in predicted values (Figure 3-3). In the centre-north the simulated potato yields were much lower than the observed yields. For the areas in the centre-south, on the other hand, the simulated yields were higher than the observed yields. The differences are because the spatial variability in observed yields is, besides variability in weather and soil data, due to the variability in management practices (e.g. fertilization). Whereas, the spatial variability simulated by the different approaches was the result of variability in weather and soil characteristics only. Moreover, the differences might be explained by the low sampling density of the soil survey in the area, or could not be explained by physical variables and therefore must be explained by other causes such as pest and diseases. Although, regional patterns of crop yield generated by different procedures (i.e. different approaches and different supports) were similar. However, a higher agreement was found for the CI approach, increasing with increasing support.

The spatial dependency of the yield maps generated by the CI and IC approaches at 100 m was characterized by a nugget-to-sill ratio of 0, and a range more than 3 km. A decrease in variance (from a nugget-to-sill ratio ≈ 41% in soil properties to 0 in the CI and IC maps) signifies a decrease of the degree of heterogeneity which is caused by the interpolation part of the CI and IC approaches. It is expected that the smoothing effect that results from interpolation (Goovaerts, 1997), results in reduced spatial variability of (Van Bodegom et al., 2002; Bouma et al., 1996), with unknown implications for the simulation results. This smoothing property of kriging is also apparent in Figure 3-3. The large range with respect to the study area indicates that there is large spatial dependency in each map. Moreover, the

Moran's I values for all maps of the different procedures were positive, significant (p = 0), and showed large spatial dependency in each of them. For comparison, Moran's I is 0.99 for the CI approach at 100 m, 0.97 for the IC approach at 100 m, 0.92 for the CI approach at 400 m, and 0.71 for the IC approach at 400 m.

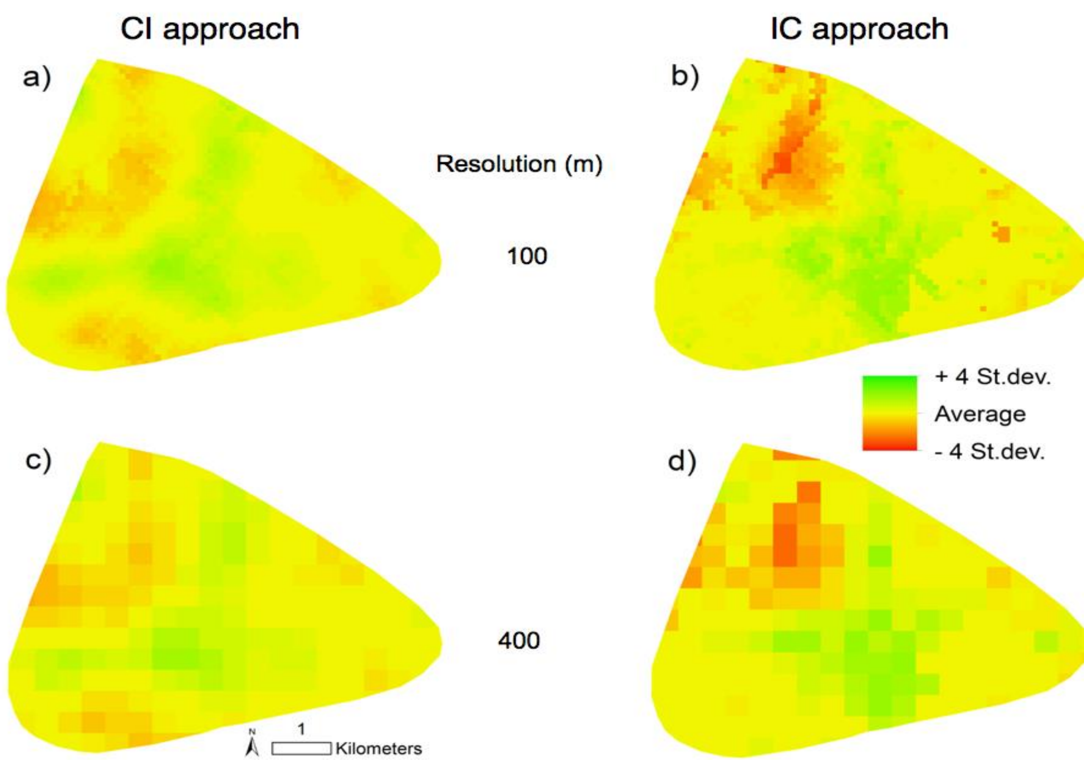


Figure 3-3: Maps of difference between interpolated, observed yield and the CI approach (left); and the IC approach (right) at supports of 100 m and 400 m in the Carchi study area.

Regional patterns of crop yield generated by different procedures (i.e. different approaches and different supports) were similar, as shown by different indicators including the semivariogram parameters (i.e. nugget-to-sill ratio and range), the Moran's I, and visually. This was expected, because (i) the area is covered by relatively young volcanic ash, and the resulting maps of soil properties (interpolated from 256 soil profiles) demonstrated large spatial dependency; (ii) there is a gradual trend in weather conditions; and (iii) spatial management variability was not considered in this study.

3.4 Conclusions

The CI and IC approaches were evaluated by comparing their outcomes to observed yields in the Carchi study area. These approaches differ with respect to the sequence of model calculation and interpolation. Results demonstrate that the order of calculations and interpolation was of major importance, while the aggregation had minor effect on the spatial pattern of potato yield. The former is probability due to the non-linearity of CGSM and the difference in the spatial dependency of individual inputs. The latter is probably due to the absence of local extremes, which is due to the gradual trends in soil properties in the volcanic ash soils of Carchi (being a result of the soil forming processes, but also a consequence of the interpolation method, kriging). The RMSD in the normalized yields was 0.79 for the CI approach and 0.99 for the IC approach at 100 m. For the aggregation to 400 m, the RMSD was 0.74 for the CI approach and 0.99 for the IC approach. The spatial comparison of regional patterns of crop yield shows that regional yield patterns generated by different procedures (i.e. different approaches and different supports) were similar, as shown by different indicators including the semivariogram parameters (i.e. nugget-to-sill ratio and range), the Moran's I, and visually. While, non-spatial comparisons of different yield patters in terms of RMSD showed better performance of the CI approach than the IC approach. From an uncertainty propagation and variability point of view it is in general preferable to calculate first before interpolation.

4 Model suitability to assess regional potato yield patterns in Northern Ecuador

A wide range of scenario studies aiming at rural development require regional patterns of crop yield. This study aims to evaluate three different modelling approaches for their suitability to assess regional potato yield patterns. The three model approaches include (1) an empirical model; (2) a process-based crop growth simulation model; and (3) a metamodel derived from the crop growth simulation model. Scenario studies have specific requirements for these modelling approaches including (1) their ease to use, (2) a realistic sensitivity, (3) the relevance in terms of generating the desired system property, and (4) their credibility in producing recognizable plausible outputs for stakeholders. The modelling approaches were applied to assess patterns of potato yields in a major production area in northern Ecuador. All three modelling approaches require significant expert knowledge for their development and calibration. However, after this initial phase, the empirical model and the metamodel are very easy to use and transparent. However, their application domain is limited to the case study area. The application of the crop growth simulation model remains complex and the model functions as a black box. The results show that regional patterns of potato yield are determined by a limited number of variables. The sensitivity of all three modelling approaches to weather variables and water holding capacity suggest that the potato production in the area is constrained by water availability and temperature. All models generate similar yield patterns. However, the empirical model derives quality adjusted potato yields that correlate highly to the observed yields, whereas the crop growth simulation model and the derived metamodel produce potential, water and nutrient limited yields. Scenario studies may require yield patterns at different levels of resolution. All results could be aggregated to different resolutions but in general the patterns remained very similar. All three modelling approaches were capable to reproduce the observed regional pattern of potato yield and are therefore considered to be credible. In analysing the effect of spatial aggregation on the performance of the modelling approaches, the results show that aggregation improves the overall correspondence between model output and interpolated, observed yields. It can be concluded that the various modelling approaches have their unique value. They are therefore complementary to each other for the interpretation of the observed patterns. The patterns themselves do not vary much and as such the most convenient modelling approach can be selected (based on available expertise and data).

Based on: Soltani, A., Stoorvogel, J.J. and Veldkamp, A. 2013. Model suitability to assess regional potato yield patterns in Northern Ecuador. European Journal of Agronomy, vol. 48, 101-108.

4.1 Introduction

Nowadays more and more scenario studies are used to explore future options for land use and agriculture (Alcamo, 2008; EEA, 2006). Well known global examples are the Global Environment Outlook (UNEP, 2002) and the Millennium Ecosystem Assessment (MEA, 2005). These large scale scenario studies involve stakeholders only in the development of storylines. In national and regional studies stakeholders can be more actively involved during scenario development by jointly developing scenarios with modellers but also in the execution and interpretation of the scenarios (Van Vliet et al., 2010). In order to involve stakeholders more effectively in a participatory modelling exercise, simplified models are required that allow stakeholders to learn and make informed decisions. It is therefore important to develop simplified models that are easy to handle and that display a realistic sensitivity to the relevant input parameters (Antle et al., 2010). Alcamo and Henrichs (2008) identify four criteria to evaluate the quality of scenarios: relevance, credibility, legitimacy and creativity. Of these four criteria, 'relevance', i.e. do they link to stakeholders needs, and 'credibility', i.e. are the outputs recognizable from the present and plausible, are relevant for the models used. This leaves us with four criteria that model approaches used in participatory scenario development should fulfil: (i) their ease to use (user friendliness), (ii) a realistic sensitivity to input variables (sensitivity), (iii) their relevance for producing the desired system property (relevance), and (iv) their credibility in producing recognizable plausible outputs for stakeholders (credibility).

Current and future yield patterns (under a range of scenarios) at different levels of aggregation are important system properties for many regional studies (Bouma et al., 2007). Accurate information on regional patterns of yield is important for commercial interests (Jagtap and Jones, 2002), strategic agricultural planning (Lobell and Ortiz-Monasterio, 2007), public policy formulation and application (De Wit et al., 2005; Wassenaar et al., 1999), and agricultural scientific innovation (Williams et al., 2008). Different modelling approaches to assess regional yield patterns exist using empirical models, process-based crop growth simulation model (CGSM), and metamodels of the CGSM.

Empirical models describe the interaction between observed crop yields (from e.g. survey data) and a range of explanatory (environmental and management) factors (e.g. Lobell et al., 2008). Empirical models have been used widely to estimate crop-yield patterns (e.g. Poudel and Kotani, 2012; Akinbile and Yusoff, 2011; Quiroga and Iglesias, 2009). The strength of empirical models is that they capture the effect of a wide range of factors that determine actual yields. Furthermore, they only require input data for variables that are selected to be relevant for the region or crop of interest (Lobell and Burke, 2010; Landau et al., 2000). However, these empirical models do not describe the underlying mechanisms explicitly and, therefore; they cannot be expected to perform well outside their calibration domain (Challinor et al., 2009, 2004). An alternative modelling approach to assess spatial patterns of crop yields is the application of a mechanistic CGSM (e.g. Xiong et al., 2008; Launay and Guérif, 2003; Faivre et al., 2000). These models have been designed to simulate crop yield in response to environmental and management factors based on the underlying physiological mechanisms (Saarikko, 2000). The application of CGSM requires experimental data for calibration. The mechanistic character of the models makes them more generic (compared to empirical models) allowing an application outside their calibration domain (within certain boundary conditions). However, CGSMs are only available for a limited number of crops, they do not include all yield limiting factors, they require highly detailed input data, and are often a black box to many users.

To resolve some of the issues related to data requirements and complexity of the CGSMs, a metamodel can be derived from the CGSM (Kleijnen and Sargent, 2000; Barton, 1998). Initially, a metamodel requires similar data as the original process based crop growth simulation model for its development. However, during the development key variables are selected that are required for its application. As such a metamodel is based on the crop growth simulation model, the problem of excluding some yield determining factors is not solved (Donatelli et al., 2010), nor is the problem of having calibration data. These are still issues that the original crop growth simulation model should address (Ewert et al., 2002; Brown and Rosenberg, 1997) before a metamodel can be derived. The application and performance of the different modelling approaches for assessing regional patterns of crop yields has rarely been investigated and evaluated in a single case study. This study aims to evaluate the three different modelling approaches for their potential use in participatory scenario development in terms of user friendliness, sensitivity, relevance, and credibility. The analysis was carried out for the potato system in Carchi in the Ecuadorian Andes.

4.2 Materials and methods

4.2.1 Study area

The Carchi Province is located in the Northern part of the Ecuadorian Andes (Figure 4-1). The study focused on an area of 36 km^2 in the eastern part of the province located at 77°50' Western longitude and 00°37' Northern latitude. Altitudes range between 2750 and 3450 m above sea level. Average annual rainfall varies between 950 and 1300 mm yr^{-1}. Being located close to the equator there is virtually no change in average monthly temperature ranging from 9 to 12 °C. The area is covered by relatively young volcanic ash deposits in which volcanic ash soils with their typical thick (about 120 cm) black A-horizon, high organic matter content (more than 4.5%), and high infiltration capacity prevail. Climatic conditions become colder and more humid with increasing altitude. At the same time, soil fertility increases with altitude with younger ash deposits and higher organic matter contents. The agricultural system is dominated by the production of potatoes and milk mostly situated on the steep Andean hillsides. The potato farming system is intensive and commercial with yields of up to 21 t ha^{-1} as a result of the favourable agro-ecological conditions in combination with the access to national and international markets (Crissman et al., 1998). The intensive and continuous production in the area does not only result in a high productivity but also in a high pest and disease pressure. Therefore, farmers use significant amounts of pesticides resulting in serious human health and environmental risks (Cole and Mera-Orcés, 2003). The intensive, commercial production of potatoes also results in a number of environmental threats such as tillage erosion and pesticide leaching. The demand for potato continues to increase. As a result potato cultivation is pushed to less favourable areas at higher altitudes and with higher erosion risk. This results in a decrease of the natural alpine páramo vegetation. There is an increasing call for participatory scenario studies in the area to deal with the problems of human health, environmental degradation, and rural development (Sherwood, 2009). These scenario studies require a better understanding of the agricultural system. Yield maps play an important role in the discussion making the study area a suitable case. Crissman et al. (1998) give a full description of the Carchi study site.

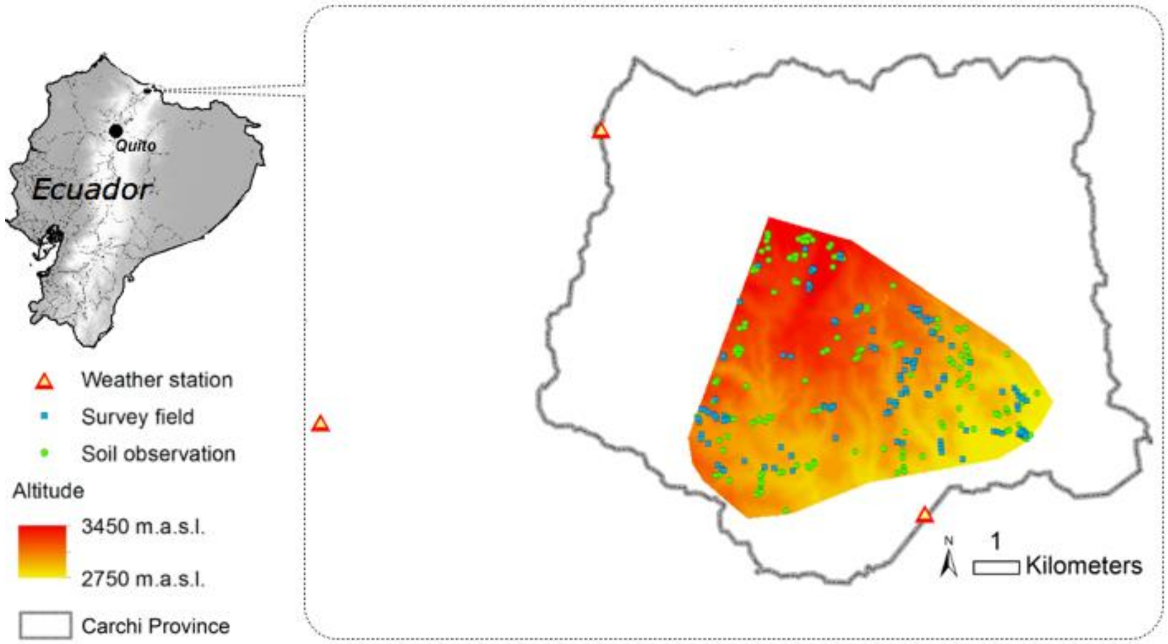


Figure 4-1: Overview of the Carchi study area in Northern Ecuador showing the altitude, the survey fields, the soil observations, and the weather stations.

4.2.2 Data and preprocessing

This study uses yield data collected during a 2-year dynamic survey including 40 farms with a total of 187 agricultural fields with 202 observations of potato yields (Figure 4-1; Crissman et al., 1998). The survey includes the detailed registration of crop yields and agricultural management such as planting date and fertilizer applications. Different potato varieties are grown in the study area. To overcome this variability in potato varieties, the yield data are expressed as quality adjusted potato yield based on the relative price levels of the different potato varieties (Crissman et al., 1998). In the Carchi study area, the potato farming system is intensive and commercial (Crissman et al., 1998). As the different potato varieties are planted throughout the year in the region mean the survey data covered several cropping cycles of five months each.

Soils are described by 256 soil profiles within the study region by Meyles and Kooistra (1997) (Figure 4-1). For each soil profile average soil properties over the top 50 cm were calculated. Subsequently, soil properties were interpolated using kriging to create a continuous surface. A digital elevation model (DEM) based on the 1:50,000 topographic maps was available for the area (100 m grid size, 2.5 m vertical resolution). Slope was derived from this DEM. Weather data are recorded at three meteorological stations around the study area including daily rainfall, minimum and maximum temperature, and solar radiation (Figure 4-1). The daily weather data were interpolated between these three meteorological stations using a digital elevation model assuming a linear relationship with altitude. Daily weather data were aggregated to yearly data for use by the empirical model and the metamodel. As the different potato varieties are planted throughout the year in the region without a clearly defined growing season, mean yearly rainfall and temperature were calculated. Due to the extreme topography in the Ecuadorian Andes, there is significant spatial variability in weather conditions. Farm management data from the survey showed a large variation in terms of planting date, fertilization, potato variety, and pesticide management. However, management differences did not show a clear spatial autocorrelation. Therefore, management variability was not considered in this study. Table 4-1 lists the total set of input variables that were considered for this study.

Table 4-1: The total set of variables; √ indicates whether or not the variable is tested in the particular model approach

Variables	Description	Empirical model	CGSM	Metamodel
<u>Topography</u>				
DEM	Elevation (m.a.s.l.)	√	-	-
Slope	Slope (%)	√	-	-
Aspect	Aspect (°)	√	-	-
<u>Weather</u>				
Tmax	Annual mean of maximum temperature (°C)	√	-	√
Tmin	Annual mean of minimum temperature (°C)	√	-	√
Rain	Annual mean of rainfall (mm d^{-1})	√	-	√
SRAD	Annual mean of solar radiation (MJ m^{-2} d^{-1})	√	-	√
D.Tmax	Daily maximum temperature (°C)	-	√	-
D.Tmin	Daily minimum temperature (°C)	-	√	-
D.Rain	Daily rainfall (mm d^{-1})	-	√	-
D.SRAD	Daily solar radiation (MJ m^{-2} d^{-1})	-	√	-
<u>Soil</u>				
SDUL	Water content at field capacity (cm^3 cm^{-3})	√	√	√
SLLL	Water content at wilting point (cm^3 cm^{-3})	√	√	√
WHC	Water holding capacity (cm^3 cm^{-3})	√	-	√
SSAT	Water content at saturation (cm^3 cm^{-3})	√	√	√
SLOC	Organic carbon (%)	√	√	√

SLCL	Clay (%)	√	√	√
SSKS	Saturated hydraulic conductivity (cm h^{-1})	√	√	√
SBDM	Bulk density (cm h^{-1})	√	√	√
SLSI	Silt (%)	√	√	√
SLCF	Coarse fraction (%)	√	√	√
SLNI	Total nitrogen (%)	√	√	√
SLHW	pH in water	√	√	√
SLHB	pH in buffer	√	√	√
SCEC	Cation exchange capacity	√	√	√
SRGF	Root growth factor	√	√	√
Interactions				
Rain x Tmin	Interaction of Rain and Tmin	√	-	√
Rain x Tmax	Interaction of Rain and Tmax	√	-	√
WHC x Tmin	Interaction of WHC and Tmin	√	-	√
WHC x Tmax	Interaction of WHC and Tmax	√	-	√
WHC x Rain	Interaction of WHC and Rain	√	-	√
$Tmax^2$	Square of Tmax	√	-	√
$Tmin^2$	Square of Tmin	√	-	√
10log(Rain)	The logarithm of Rain	√	-	√

4.2.3 Interpolated yield data

Spatial autocorrelation of the observed potato yields was studied through an analysis of the semivariogram. The yields were interpolated using kriging to create a yield map. The quality of the map was evaluated by a cross validation. The cross validation involved consecutively removing a data point, interpolating the value from the remaining observations and comparing the predicted value with the measured value (Mueller et al., 2004). The kriging performance was validated in terms of the CV-RMSD. The CV-RMSD is defined as the root mean squared difference normalized to the average of the observed values and calculated as:

$$CV - RMSD = \frac{\sqrt{\sum_{i=1}^{n}(\hat{x}_i - x_i)^2/n}}{\bar{x}} \quad (4.1)$$

Where x_i is the observed yield, $\hat{x}_i$ the interpolated, observed yield for the cell containing observation i, $\bar{x}$ is the average observed yield for the area, and n is the number of observations.

4.2.4 Modelling yield patterns

Empirical model

An empirical model was created to describe the interaction between crop yield and the various explanatory variables in Table 4-1. To construct an empirical model, the yield observations were split into a calibration (102 fields) and a validation (100 fields) dataset. We deliberately choose variables that are also available at wide temporal scales. Because we know from theory that some variables are non-linearly related to crop yields, various transformations were included. For temperature we included a squared term, to allow the regression to pick up the fact that temperature has an optimum; for precipitation we included a log transformation, to prevent that the signal from normal rain variability becomes obscured by extreme rainfall events. Furthermore, we included several interactions (see Table 4-1). These were included to account for the possibility that, e.g. water holding capacity becomes a more important determinant of crop yield in areas where rainfall is low. A Pearson correlation matrix was calculated to indicate the degrees of colinearity between all explanatory variables. The most significant independent variables for predicting potato yields were selected by means of a backward elimination of the variables with the lowest statistical significance. The results of the final model obtained by applying the regression model to the validation dataset of explanatory variables were compared with the yield observations. The results of the validation were expressed as the CV-RMSD similar to Eq. (4.1) and a coefficient of determination (R^2). The coefficient of determination was calculated as 1 − SSE/SST, whereby SSE is the sum of squares of residuals, and SST is the total sum of squares. A map of potato yields was created using the empirical model in combination with the maps of the relevant explanatory variables.

Crop growth simulation model

The SUBSTOR-potato model (Ritchie et al., 1995) is a mechanistic crop growth simulation model that simulates potato yield as a function of environmental and management factors. This CGSM is available within the Decision Support System for Agro-technology Transfer (DSSAT) (Jones et al., 2003). The SUBSTOR-potato model simulates the physical, chemical, and biological processes in the plant and its associated environment. Bowen et al. (1999)

and Clavijo (1999) calibrated and validated the SUBSTOR-potato model for Andean conditions using experimental data from the region. Table 4-1 lists the total set of variables that were considered in the application of the CGSM. For the crop growth simulation model representative management data are used with a nitrogen application of 168 kg ha^{-1} $season^{-1}$ planted on February 15. The model was run for each of the grid cells to create a map of the expected potato yields using interpolated daily weather data, interpolated soil properties, and representative management data.

Metamodel

A metamodel was derived from the calibrated SUBSTOR-potato model. Meyles and Kooistra (1997) provided complete soil profile descriptions for 256 sites in the Carchi region. Potato yields were simulated using the CGSM for these 256 points. The dataset with simulated yields was split into a calibration (130 observations) and a validation dataset (126 observations). The metamodel was obtained by relating model input to model output of the calibration dataset following the same statistical procedures as used during the development of the empirical model. The results of the final model obtained by applying the regression model to the validation dataset of explanatory variables were compared with the simulated yield. The results of the validation were expressed as the CV-RMSD similar to Eq. (4.1) and a coefficient of determination (R^2). A map of potato yields was created using the metamodel in combination with the maps of the relevant explanatory variables.

4.2.5 Model comparison

Studies typically evaluate yield patterns on the basis of a range of observation points using statistical techniques like the root mean square difference (Akinbile and Yusoff, 2011; Quiroga and Iglesias, 2009; Xiong et al., 2008; Launay and Guérif, 2003). However, the application of the model-based approaches for the analysis of participatory scenarios requires different characteristics in terms of, e.g. user friendliness and sensitivity. Therefore, we compared the three different modelling approaches for their potential use in participatory scenario development in terms of their user friendliness, sensitivity, relevance, and credibility.

The user friendliness of the models to predict yield patterns was compared in terms of the number of input variables used, computation time, and transparency. The sensitivity of the models to predict pattern yield was compared by showing the models sensitivity to different explanatory variables and respective coefficient of the different variables. The models relevance was compared by analysing the unit of analysis (i.e. actual yield or potential yields) and the effect of scale of the predicted yield pattern. Many scenario studies are not interested in the results at the field level, but require more general patterns of yields with supports larger than the field. Therefore, all yield maps (observed and model-based) were aggregated to higher aggregation levels of 200, 300, 400, 500 and 600 m resolution. Subsequently, the model-based yield maps were compared to the interpolated, observed yields with the aim of analysing models relevance by producing the yield patterns at support resolutions larger than field in terms of root mean squared difference (RMSD). The RMSD is calculated as:

$$RMSD = \sqrt{\frac{\sum_{i=1}^{n}(\hat{x}_i - x_i)^2}{n}} \qquad (4.2)$$

where x_i is the interpolated, observed yield, $\hat{x}_i$ the model-based yield for cell i, and n is the number of cells.

The credibility of the models was analysed by comparing the model-based yield maps to the interpolated, observed yield map, evaluated visually and in terms of the RMSD. Although, the comparison of the predicted patterns in potato yield to the interpolated, observed yields is not a true validation. Most of the time real patterns of yield are unknown and we will have to describe the spatial pattern through interpolation. Due to the different potato varieties, the yield maps based on the actual observations are expressed in quality adjusted potato yields. However, the CGSM and the metamodel provide nutrient limited, potential yields. Given the fact that we are interested in patterns in the potato production and to make the maps inter-comparable, the four maps were normalized as $(\hat{Y} - \bar{Y})/Y_{sd}$ with $\hat{Y}$ being the estimated yield (interpolated, observed yield or modelled yields), $\bar{Y}$ the average yield over the entire map, and Y_{sd} the standard deviation of the yield for the map.

4.3 Results and Discussions

4.3.1 Observed yields

Yield maps were made based on interpolation of the 202 data points. The semivariogram of the observed yields showed a nugget- to-sill ratio of 58% indicating a moderate spatial autocorrelation. The yields were interpolated with ordinary kriging. The cross validation revealed a CV-RMSD of 17%. Although the yield map explains part of the variation, a large part of the variation remains unexplained. The large nugget can be caused by a short distance variation in the yields caused by differences in management. The spatial variation in yield is due to variation in weather, soil properties, and management data. There is a limited short-distance variation of soil properties and weather condition. As the area is covered by relatively young volcanic ash and there is a general trend in weather condition based on altitude. Therefore, management differences are considered to be responsible for the unexplained variance in yields (e.g. fertilization, pesticide use). The resulting map (Figure 4-2a) demonstrates that the highest yield levels are attained in the western part with altitudes between 3000 and 3300 m.a.s.l. These areas are considered to be the prime potato growing region. They are dominated by young volcanic ash soils, but they also have enough rainfall and are relatively cool. The results demonstrate a yield decrease towards warmer and dryer conditions that coincides with lower elevation in the Andean mountain range. Potato growth is constrained by the cold temperatures in areas above 3300 m.a.s.l. Moreover, these areas are often cloudy with lower irradiation and rainfall is very high. At lower elevations, approximately 2700–3000 m, lower yields coincide with less rainfall and older, less fertile soils.

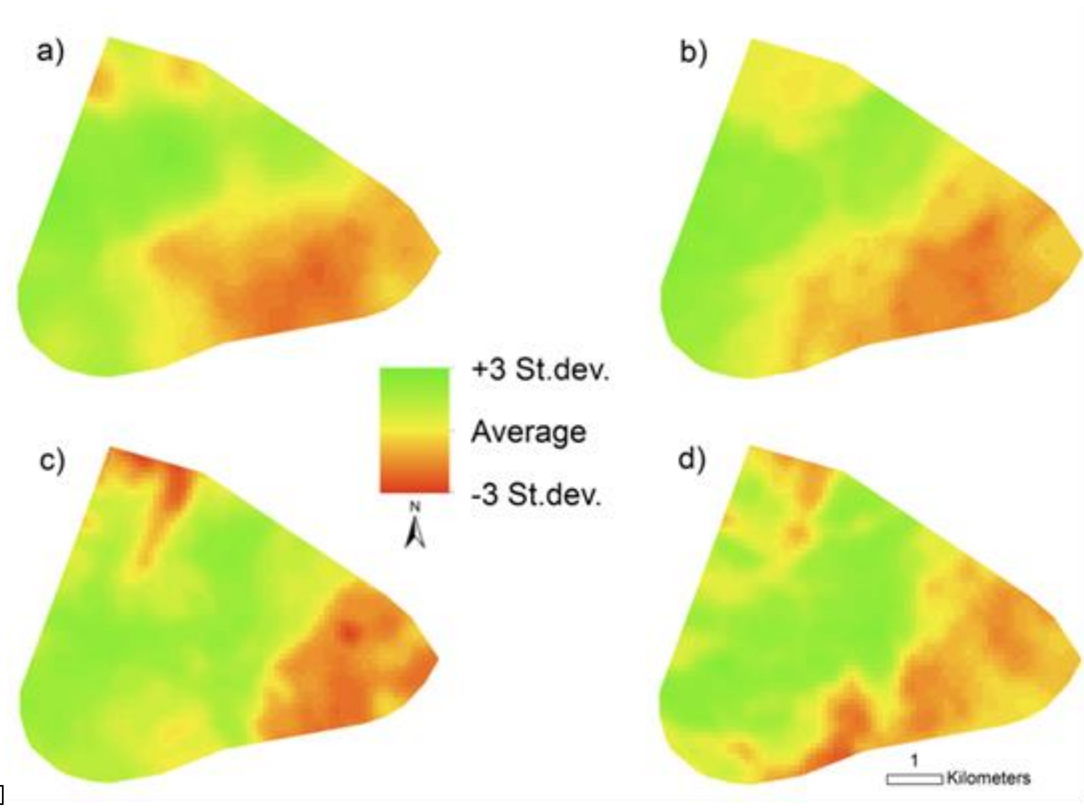


Figure 4-2: Maps of normalized potato yield in the Carchi study area based on: (a) interpolated, observed yields, (b) empirical model, (c) crop growth simulation model, and (d) metamodel.

4.3.2 Modelling yield patterns

Empirical model

A linear regression that related the explanatory variables of Table 4-1 to the observed yields resulted in the following model (calculated potato yield for the empirical model is in quality adjusted, actual yields):

$$Yield = -5.1 + 27.8\ WHC + 0.3\ Tmin$$

This model described around 43% (=R^2) of the observed potato yield with a CV-RMSD of 9% for the calibration dataset. The model predicted 36% (=R^2) of the observed potato yield for the validation dataset with a CV-RMSD of 12%. According to this model, yields are higher on soils with higher water holding capacity, which is related to plant available water. Yields increase with increasing annual minimum temperature, which can probably be ascribed to a reduced risk on frost damage. From Table 4-2, it can be seen that annual minimum temperature is strongly correlated to annual maximum temperature and rainfall, implying that this annual minimum temperature may also serve as a proxy for annual maximum temperature and rainfall. The model is sensitive to soil water holding capacity and temperature. It is not surprising that soil fertility is not included. The area is covered by volcanic ash soils with their typical thick (about 120 cm) black A-horizon, and high organic matter content (more than 4.5%). Moreover, high input agriculture characterized by a significant fertilizer input prevails in the area. The normalized map created by the empirical model is shown in Figure 4-2b. The map shows the highest yield levels in the western part with altitudes between 3000 and 3300 m.a.s.l.

Crop growth simulation model

The CGSM simulated the nutrient limited potato yield using daily weather data, soil properties, and representative management data in the validation dataset. This resulted in a map of simulated potato yields that was normalized as displayed in Figure 4-2c. The resulting map demonstrates that the higher yield levels are attained in the western part, where altitudes are between 3000 and 3300 m.a.s.l.

Metamodel

The metamodel was created by running a regression between the input variables and the potato yield predicted by the SUBSTOR-potato model for 256 points for which complete soil profile descriptions were available. The best metamodel to emulate the potato yield estimates (in t ha^{-1} $season^{-1}$) result of the CGSM is:

$$Yield = - 10.8 + 20.4\ WHC + 0.5\ Rain \times Tmin$$

The results of the metamodel and the CGSM had an R^2 of 48% with a CV-RMSD of 17% for the calibration dataset. The metamodel predicted 41% (=R^2) of the potato yield estimates by the CGSM for the validation dataset with a CV-RMSD of 21%. According to this model, yields are higher on soils with higher water holding capacity. In the study area, yield increase towards cooler and wetter conditions. Considering the fact that interactions are known to exist therefore annual rainfall and minimum temperature interactions were tested and improved the results of the metamodel. In this model only water availability and weather condition (the interaction of annual rainfall and minimum temperature) are included. The normalized, metamodel map is shown in Figure 4-2d. The resulting map demonstrates that the highest yield levels are attained in the western part, where altitudes are between 3000 and 3300 m.a.s.l.

4.3.3 Model comparison

User friendliness

It can be observed from Table 4-3, that the empirical model and the metamodel require less input variables (2 and 3 respectively) compared to the CGSM (18) to estimate regional patterns of potato yield. Comparison of the relative computation time under the same conditions (i.e. CPU, memory and software) provides useful information for choosing a more efficient modelling approach (Guo et al., 2010). We record the average processing time for each modelling approach to create a map of potato yield at 100 m resolution, and the results are shown in Table 4-3. The empirical model and the metamodel prove to be relatively simple and fast, while the CGSM requires more computation time.

The empirical model and the metamodel are linear regressions that explicate the relationships between potato yield and relevant significant variables, valid in that context and at that scale. Such regressions are simple and intuitively easy to comprehend by stakeholders. The CGSM is a more complex model that is less transparent for non-experts and acts like a black box for non-expert users. But in terms of flexibility, it provides more options. Giving the model users the opportunity to contribute and challenge model assumptions before results are reported also creates a sense of ownership (Korfmacher, 2001). However, this requires transparent models that are well understood by the end-users. Therefore, when used directly by stakeholders empirical and metamodel approaches are the suitable choice. To conclude, the empirical model and metamodel where key driving variables are selected in an early stage of the research have the advantage of greater simplicity and transparency. In addition, they require less computation time compared to CGSM. The empirical model is easiest to use followed by metamodel. The CGSM requires too much data to be ways to use in a part scenario development. Nevertheless, statistical procedures and correlations between variables may make the estimation of empirical and metamodels difficult to understand.

Table 4-2: Pearson correlation coefficient between variables in the empirical and metamodel approach

	SBDM	SCEC	SDUL	SLCL	SLHB	SLHW	SLLL	SLNI	SLOC	SLSI	SSKS	SSAT	Tmax	Tmin	Rain
SBDM	1														
SCEC	-0.44	1													
SDUL	-0.45	0.86	1												
SLCL	0.19	-0.08	-0.35	1											
SLHB	0.77	-0.47	-0.63	0.49	1										
SLHW	0.79	-0.52	-0.66	0.62	0.88	1									
SLLL	-0.47	0.85	1	-0.36	-0.64	-0.66	1								
SLNI	0.06	0.33	0.52	-0.58	-0.31	-0.42	0.53	1							
SLOC	0.15	0.35	0.51	-0.51	-0.20	-0.33	0.51	0.96	1						
SLSI	0.41	0.08	0.04	0.21	0.34	0.26	0.02	0.40	0.49	1					
SSKS	0.68	-0.84	-0.89	0.32	0.73	0.78	-0.88	-0.42	-0.38	0.03	1				
SSAT	0.41	0.13	-0.07	0.38	0.70	0.56	-0.10	-0.22	-0.11	0.24	0.23	1			
Tmax	0.61	-0.70	-0.77	0.27	0.73	0.74	-0.74	-0.52	-0.47	-0.11	0.83	0.36	1		
Tmin	0.61	-0.70	-0.77	0.27	0.73	0.74	-0.74	-0.52	-0.47	-0.11	0.83	0.36	1	1	
Rain	-0.61	0.69	0.76	-0.27	-0.73	-0.74	0.73	0.53	0.47	0.11	-0.82	-0.37	-1	-1	1

Table 4-3: The evaluation of three different modelling approaches (an empirical model, a crop growth simulation model (CGSM), and a metamodel) to assess potato yield patterns in the Carchi study area

Criteria		Empirical model	CGSM	Metamodel
User friendliness	Number of variables required	2	18	3
	Computation time (S)	45	600	45
	Transparency	yes	no	Yes
Sensitivity	Explanatory variables	Obvious	Requires sensitivity analysis	Obvious
	Application domain	Similar agro-ecology	Wider range of conditions	Similar agro-ecology
Relevance	Yield unit	Actual yield	Potential yield	Potential yield
Credibility	RMSD	0.61	0.99	1.05

Sensitivity

From the resulting models it can be seen that regional patterns of potato yield are determined by a limited number of variables. The empirical model and metamodel demonstrate the sensitivity to soil water holding capacity and weather conditions as important explanatory variables, except that metamodel picked up the interaction of annual rainfall and minimum temperature while the empirical model picked up annual minimum temperature. Moreover, the weather variables in the empirical and metamodel allow for their potential use in climate change scenarios. In our specific case study soil fertility is not included in the empirical model and the metamodel. This seems a logical consequence of the relative fertile soils in combination with the high input agriculture. The explanatory variables in the empirical model and metamodel are obvious. In the case of CGSM, a sensitivity analysis is required to obtain sensitivity information (Table 4-3). The development of a metamodel could be a good alternative for the sensitivity analysis to assess the key variables of the CGSM.

At the regional level other yield determining factors such as pests and diseases may play a role, which are not accounted for in CGSM and the derived metamodel. While, empirical models implicitly consider these other yield-limiting factors when empirical data are available. This could explain the slightly better performance of the empirical model with a RMSD of 0.61 as this model is calibrated on the observed potato yields. The fundamental limitation of any empirical model is that it is not valid outside its calibration domain. This seriously hampers its usefulness for scenario studies (White, 2009). The strength of the CGSMs is that impacts over a longer time frame can be simulated, taking into account many factors in a way that would not be possible using empirical models and metamodels (Lobell and Burke, 2010; Bouman et al., 1998).

Relevance

The models' relevance was compared by analysing the unit of analysis and effect of scale of the predicted yield pattern. The empirical model has the potential to consider other yield determining factor such as pests and diseases and therefore provide actual yields in contrast to the potential yield provided by the CGSM and the metamodel (Table 4-3). At the level of small grid cells substantial errors might be found, preventing a direct interpretation of the model outcomes at this level. However, the analysis was carried out aiming at regional patterns of potato yield in Carchi with regards to the biophysical variables rather than evaluating the outcome of each individual basis cell. Moreover, scenario studies often require results at supports larger than a field support. Therefore, all yield maps (observed and model-based) were aggregated to different levels of resolution with the aim of analysing the effect of spatial aggregation on the performance of the modelling approaches.

The results show that increasing the level of spatial aggregation increased the similarity between simulated yield patterns and interpolated observed yield, as illustrated in Figure 4-3. This is confirmed by studies of Kok and Veldkamp (2000) and Verburg et al. (1999). In their model validation they found that deviations between modelled and actual land use at the cell level can be considerable, but that very good agreement was found at the higher level such as agro-ecological zone or district.

In this study, the rates of decreasing RMSD with higher aggregated levels were similar for the different modelling approaches and in most cases resulting in a linear decline of 15–30%. The decreasing RMSD with increasing aggregation was expected as the variability of data will decrease and local extremes will be levelled out (Baron et al., 2005; Hansen and Ines, 2005; Easterling et al., 1998). In this study we aggregated the yield maps to five aggregations levels. However, at different scale levels different explanatory variables may play a role (De Koning et al., 1998). A more proper analysis should include separate model estimation at each of the hierarchical scale levels rather than an aggregation of the final results. Therefore, some caution has to be taken when interpreting the results of such an analysis.

Credibility

In the current study, the maps of the different modelling exercises demonstrate a good correspondence with the survey data, evaluated visually and in terms of RMSD. The different modelling approaches properly identified the high-productivity regions in the western part, where altitudes are between 3000 and 3300 m.a.s.l. as well as the low-productivity regions in areas above 3300 m.a.s.l., and at lower elevations, approximately 2700–3000 m (Figure 4-2). The RMSD values for the difference of the three model-based maps from the map of observed potato yields show that the yield differences were lowest for the empirical model, showing a RMSD of 0.61. The RMSD in the normalized yields was highest for the metamodel, showing a RMSD of 1.05. The CGSM shows a more modest difference in the yields, showing a RMSD of 0.99 (Table 4-3). The empirical model outperforms CGSM and metamodel in being better able to analyse the regional pattern of yield. This might be also explained by that part of the variation that could not be explained in the CGSM and metamodel and therefore must be explained by other causes such as pest and diseases.

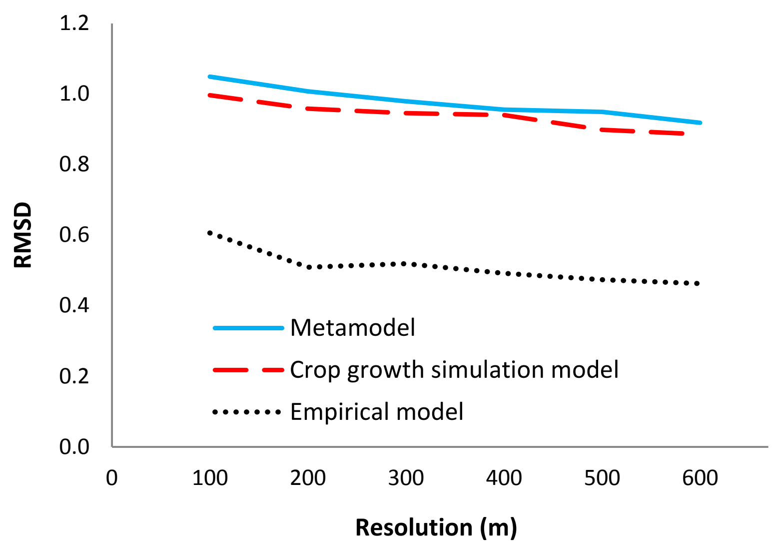


Figure 4-3: Root mean squared differences at the different levels of aggregation comparing model-based approaches to the map of observed potato yields in the Carchi study area.

4.4 General discussions

Previous integrated assessment studies for the study area showed the importance of the variation of yield differences in the study area in a range of econometric production models (e.g. Stoorvogel et al., 2004; Antle and Stoorvogel, 2006). The integrated assessment models were used in participatory scenario analysis to deal with environmental issues like pesticide leaching in combination with rural development (Sherwood, 2009). One of the key constraints of the modelling approach was the complexity of the models. The calibration but also the actual subsequent analysis of the mechanistic models for crop growth and pesticide leaching was recognized as a serious limitation. This refers mainly to the user friendliness but of the mechanistic modelling approaches. In a later stage this has led to the development of a new suite of parsimonious models (e.g. Antle et al., 2010). As illustrated in this study, there is not a single optimal solution to modelling agricultural systems to assess, e.g. regional yield patterns. Since there will always be a certain level of idiosyncrasy to the case, we have to strive towards a toolbox of approaches (Bouma et al., 2007) from which the proper tool can be selected on the basis of a number of specific criteria (like user friendliness, sensitivity, relevance, and credibility). In this study, we selected different models using different calibration data (observed yields for the empirical model and experimental data for the CGSM) and at different levels of detail (e.g. CGSM vs. metamodel). We recognize that there are other methods available (see e.g. Reimer and Li, 2009). We do not give a final preference to one of the approaches. This depends on the specific study the results are being used for, but also the results were rather similar.

4.5 Conclusions

Three modelling approaches of an empirical model, a CGSM, and a metamodel were applied to assess patterns of potato yields in a major production area in northern Ecuador. All three modelling approaches require significant expert knowledge for their development and calibration. However, after this initial phase, the empirical model and the metamodel are very easy to use and transparent, although the application domain is limited to the case study area. The application of the simulation model remains rather complex and functions as a black box. The results show that regional patterns of potato yield are determined by a limited number of variables. The sensitivity of all three modelling approaches to weather variables and water holding capacity suggest that the potato production is constrained by water availability and temperature. All models generate similar potato yield patterns. The empirical model derives quality adjusted potato yields that correlate to observed yields. The crop growth simulation model and the derived metamodel produce potential, water and nutrient limited yields. Scenario studies may require yield patterns at different levels of resolution. All results could be aggregated to different resolutions but in general the patterns remained very similar. All three modelling approaches were capable to reproduce the observed regional pattern of potato yield and are therefore considered to be credible. In analysing the effect of spatial aggregation on the performance of the modelling approaches, the results show that aggregation improves the overall correspondence between model output and interpolated, observed yields. It can be concluded that the various modelling approaches have their unique value. They are therefore complementary to each other for the interpretation of the observed patterns. The patterns themselves do not vary much and as such the most convenient modelling approach can be selected (based on available expertise and data). Proper model evaluation requires different criteria including user friendliness, sensitivity, relevance, and credibility.

5 How to use crop growth models at regional scales? A case study of winter wheat yield in Western Germany

Trends and patterns in winter wheat in Western Germany were simulated using three different modelling approaches. Yield estimates by LINTUL2, a process-based model, were compared with those of a metamodel and an empirical model. Model outcomes were aggregated to administrative units for the whole of Western Germany to allow comparison with agricultural census data for validation purposes. The spatial patterns and temporal trends seem to be better represented by the empirical model (R^2= 69%, RMSE= 0.49 t $ha^{-1}yr^{-1}$, and CV-RMSE= 8%) than by the LINTUL2 model (R^2= 65%, RMSE= 0.67 t $ha^{-1}yr^{-1}$, and CV-RMSE=11%) and the metamodel (R^2= 56%, RMSE= 0.79 t $ha^{-1}yr^{-1}$, and CV-RMSE=13%). All models demonstrate a similar order of magnitude of yield prediction and associated uncertainties. The suitability of the three models used are context dependent. Empirical modelling is most suitable to analyse and project past and current crop-yield patterns while crop growth simulation models are more suited for future projections with climate scenarios. The derived metamodels are fast reliable alternatives for areas with well calibrated crop growth simulation models. A model comparison helps to reveal shortcomings and strengths of the models. In our case, a performance comparison between the three models indicated that a higher sensitivity to soil depth and winter wind speed in the LINTUL2 model and the metamodel would probably lead to better predictions. This specific conclusion is only valid for winter wheat growth in western Germany, for the used models.

Based on: Soltani, A., Bakker, M.M., Veldkamp, A., Stoorvogel, J.J. and Angulo, C. How to use crop growth models at regional scales? A case study of winter wheat yield in Western Germany. Ecological modelling (under revision).

5.1 Introduction

Process-based crop growth simulation models are a commonly used tool for future projections of crop yields within climate scenarios (Challinor et al., 2009; Lobell et al., 2008; Ewert et al., 2005; Parry et al., 2004). These models are mainly developed for the plot and field scale, requiring location-specific, spatially homogenous input data (Tao et al., 2009; De Wit et al., 2005; Van Ittersum et al., 2003; Mearns et al., 2001; Hansen and Jones, 2000). When such models are applied to larger areas (e.g. provinces or countries) and at annual time steps, there is a scaling challenge (Kok and Veldkamp, 2011; Tao et al., 2009; Saarikko, 2000). At wider spatial scales other factors than those typically used by crop growth simulation models co-determine yield variability (e.g. pests, plagues etc.). Furthermore, using aggregated input data may require recalibration of the model (Easterling et al., 2001). Also at wider temporal scales new factors may emerge that turn out to be important (e.g. technological development), which are not accounted for in crop growth simulation models (Bakker et al., 2005; Kok and Veldkamp, 2001). Furthermore, the required detailed weather data is not directly generated by future climate scenarios because they use annual or courser time steps (DDC IPCC, 2010; Janssen et al., 2009). Consequently the required high resolution data are generated by data modelling exercises using weather generators and other downscaling techniques (Qian et al., 2011; Apipattanavis et al., 2010).

That leaves us with the question how to best use data and models at regional scales. Apart from adjusting crop growth simulation models to wider scales and/or generating the required detailed input data, there are two other known solutions for solving the scaling challenge. One is replacing the crop growth simulation model by a metamodel, that can deal with less detailed data (Kleijnen and Sargent, 2000; Barton, 1998), and the second approach is using the survey data to derive an empirical model relating observed yields to environmental characteristics (Lobell and Burke, 2010; White, 2009; Veldkamp et al., 2001). A metamodel would require similar data as the original process based crop growth simulation model but instead of daily, annual average of daily weather data (Audsley et al., 2008). Moreover, in most regions, only a limited number of environmental and management factors determine crop growth (e.g. Soltani et al., 2013). As a result one can wonder whether we need the full complexity of the crop growth simulation models in those cases. However, as such a metamodel is based on the crop growth simulation model, the problem of not including factors (Donatelli et al., 2010) that play a role at wider temporal and spatial scales is not solved: these are still issues that the original crop growth simulation model should address (Ewert et al., 2002; Brown and Rosenberg, 1997), before it can be replaced by a meta model. A data-based empirical model can use all data available including other data sources depending on availability and hypothesized relationships. It is calibrated directly on the aggregated input data, and can include all kinds of factors at any available aggregation level. Their disadvantage is that extrapolation beyond the calibration range of input variables is unreliable, and the relationships used are context dependent and not process based (Bakker and Veldkamp, 2012).

This chapter compares the following three approaches to simulate and predict crop yields at wide spatial and temporal scales: 1) a crop growth simulation model, 2) a metamodel, and 3) an empirical model. The crop growth simulation model was to some extent adapted to wider spatial and temporal scales: it includes a technology development factor and it was recalibrated for spatially aggregated input data (Angulo et al., 2012). It was, however, not recalibrated for temporally aggregated weather data, nor did it include factors such as pests and plagues that become important at wider spatial scales. The metamodel is potentially able to overcome the issue of being able to use temporally aggregated data, but not the issue of including factors such as pests and diseases. The empirical model relates available input data to output data and can resolve the scale and new factor issues, but might not be reliable when used in future scenarios that will automatically exceed the calibration range. All three models will be calibrated for one time period and validated for a subsequent time period by comparison with observed yields for one case study, Western Germany. Finally, the models will be used to make a future prediction of crop yields for 2050.

5.2 Materials and methods

5.2.1 Study area

Western Germany (i.e. former West Germany) covers a wide range of agro-ecological conditions. The northwest and the north have a sea climate while the Alpine regions have a boreal climate. The average annual rainfall ranges between 200 in the East and Upper Rhine Graben and 1600 mm in the Alps; the average annual temperature ranges between 2°C in the higher Alps and 11°C in the North. Over 80% of the land is used for agriculture and forestry. Like in other modernized countries, the agricultural sector has undergone profound structural changes in the second half of the 20th century. The number of farms decreased dramatically as a result of increasing mechanization coinciding with increased productivity per hectare. Nevertheless, family farms still predominate in Western Germany (87% of all farms comprised less than 50 hectares in 1997). Arable farming is dominated by soft winter wheat (Triticum aestivum L.). Temporal averages over the period 1993-2002 of the annual winter wheat yields in the individual climate zones varied between approximately 4 t ha^{-1} in the south and southwest to 8 t ha^{-1} in the north and northeast (Figure 5-1a).

5.2.2 Data

Time series of winter wheat yields from 1983 to 2002 were obtained from the Statistisches Bundesamt Deutschland (Bakker et al., 2005) at NUTS3 level, which is the finest spatial level at which agricultural statistics are available.

Weather data were obtained from the SEAMLESS database (van Ittersum et al., 2008) for 70 climate zones in Western Germany (Andersen et al., 2010; Janssen et al., 2009) for the period 1983-2002. Data included daily data on rainfall (mm d^{-1}), maximum and minimum air temperature (°C), global solar radiation (MJ $m^{-2}d^{-1}$), wind speed (m s^{-1}), vapour pressure (hPa), and evapotranspiration (mm d^{-1}, calculated with the Penman–Monteith formula as applied by Allen et al. (1998)).

Soil characteristics at the level of so-called AgriEnvironmental Zones (Hazeu et al., 2010), which are a further refinement of the climatic zones, were obtained from the Pan European SEAMLESS database (Andersen et al., 2010; van Ittersum et al., 2008). Data included critical soil water content for transpiration reduction due to water logging, and the water content at field capacity, saturation, wilting point, and air dryness. In addition, soil depth was obtained from the Pan European Soil Erosion Risk Assessment project (contact no: QLK5-1999-01323, http://www.pesera.jrc.it). Soil depth is available at a 1 km grid covering all of Europe, and is defined as the depth to a rooting restriction (bedrock, very dense soil material or groundwater) with a maximum value of 1 m (i.e. implying no constraint for crop growth).

Technological development has also played an important role in the development of yields over time (Challinor et al., 2009; Semenov and Halford, 2009; Ewert et al., 2005). Here, we use a proxy for technological development as described in Ewert et al. (2005) to estimate yield increase due to improved varieties and crop management (e.g. pesticides and herbicides). The available yields statistics were de-trended to exclude yield increases resulting from technology development. For this purpose, yield trends were calculated for each climate zone by fitting a linear regression line through the correspondent observed yields, as described by Ewert et al. (2005). Following this approach (i.e. a linear de-trending), for each climate zone a trend in technological development was obtained by setting the initial technological development (in our case the year 1983) to e.g. 1.033, and we obtain a value of each subsequent year by multiplying the value of the previous year by 1.033. This variable is spatially explicit, showing a range between 1.033 and 1.077.

Yearly sowing and harvest dates for winter wheat were obtained from the JRC/MARS Crop Knowledge Base for 70 climate zones in Western Germany for the period 1983-2002 (JRC, 1998). These data of sowing and harvest dates were then used for the application of LINTUL2.

As a projection of climate change by the mid-21st century, we used the ensemble mean of 15 Global Circulation Models (GCMs) calculated as part of the third Coupled Model Inter-comparison Project (CMIP3) provided by the Intergovernmental panel on Climate Change (IPCC) Data Distribution Centre (DDC) (DDC IPCC, 2010). CMIP3 evaluated a range of different scenarios. In this study, we used the A1B scenario which corresponds to rapid economic growth in an integrated world where the global population reaches 9.1 billion in 2050. The A1B scenario projects for Western Germany an increase in maximum temperatures of 1.3 - 2.7°C, an increase of minimum temperatures of 0.8 - 2.2°C, a decrease in precipitation of 0.1 - 0.8 mm d^{-1}, an increase in vapour pressure of 0.08 - 0.15%, changes in wind speed between -0.8 - 0.4%, and changes in evapotranspiration between -0.1 - 0.4%. All these variables are spatially explicit, showing a general gradient from northwest to the southeast. Climate change is smallest in the northwest; towards the southeast rainfall reduces over time while all other variables increase.

Increases in CO_2 levels are likely to result in a yield increase (Erda et al., 2005; Southworth et al., 2002; Eitzinger et al., 2001). Potential negative impacts of climate change on C3 crop yields can be offset by the fertilization effect of increased CO_2 as described in (Nowak et al., 2004; Kimball et al., 2002). Angulo et al. (2012) used a simple representation of the effects of increased atmospheric CO_2 level (ppm) on winter wheat yield, using the relationship between CO_2 and radiation-use efficiency as proposed by Stockle et al. (1992). Increased CO_2 also reduces crop transpiration. A linear diminution of transpiration up to 10% for winter wheat was taken into consideration by Angulo et al. (2012), when the atmospheric CO_2 reaches 700 ppm (Ewert et al., 2002). IPCC (2001) reports a gradual increase of the average CO_2 level for the SRES A1B scenario from 374 ppm in 2002 up to 532 ppm in 2050. There is no spatial variability assumed for this variable.

All data were aggregated to the coarsest spatial level: that of the climate zone. This resulted in 70 observations on yield, as response variable, and a range of explanatory variables which are listed in Table 5-1.

Weather data were also temporally aggregated so that they could be used by the empirical model and the metamodel (which both operate with an annual resolution). Three aggregations were made: (i) by taking the annual average of daily weather data, (ii) by taking the average over the growing season (April to August), and (iii) by taking the average over winter (December-March). The winter period is relevant because winter wheat is sown in autumn and has a dormancy period throughout winter.

Table 5-1: The total set of variables; √ indicates whether or not the variable is tested in the particular model approach

Variables	Description	Empirical model	LINTUL2	Meta-model
Management data				
TD	Technological development (-)	√	√	√
S.dates	Sowing dates	-	√	-
H.dates	Harvest dates	-	√	-
Weather				
Tmax	Mean annual maximum temperature (°C)	√	-	√
Tmin	Mean annual minimum temperature (°C)	√	-	√
Rain	Mean annual rainfall (mm d^{-1})	√	-	√
SRAD	Mean annual global solar radiation (MJ m^{-2} d^{-1})	√	-	√
WS	Mean annual wind speed (m s^{-1})	√	-	√
VP	Mean annual vapour pressure (hPa)	√	-	√
ET	Mean annual evapotranspiration (mm d^{-1})	√	-	√
G.Tmax	Mean growing season maximum temperature (°C)	√	-	√
G.Tmin	Mean growing season minimum temperature (°C)	√	-	√
G.Rain	Mean growing season rainfall (mm d^{-1})	√	-	√
G.SRAD	Mean growing season global solar radiation (MJ m^{-2} d^{-1})	√	-	√
G.WS	Mean growing season wind speed (m s^{-1})	√	-	√
G.VP	Mean growing season vapour pressure (hPa)	√	-	√
G.ET	Mean growing season evapotranspiration (mm d^{-1})	√	-	√
W.Tmax	Mean winter season maximum temperature (°C)	√	-	√
W.Tmin	Mean winter season minimum temperature (°C)	√	-	√
W.Rain	Mean winter season rainfall (mm d^{-1})	√	-	√
W.SRAD	Mean winter season global solar radiation (MJ m^{-2} d^{-1})	√	-	√
W.WS	Mean winter season wind speed (m s^{-1})	√	-	√
W.VP	Mean winter season vapour pressure (hPa)	√	-	√
W.ET	Mean winter season evapotranspiration (mm d^{-1})	√	-	√
D.Tmax	Daily maximum temperature (°C)	-	√	-
D.Tmin	Daily minimum temperature (°C)	-	√	-
D.Rain	Daily rainfall (mm d^{-1})	-	√	-
D.SRAD	Daily global solar radiation (MJ m^{-2} d^{-1})	-	√	-

D.WS	Daily wind speed ($m\ s^{-1}$)	-	√	-
D.VP	Daily vapour pressure (hPa)	-	√	-
D.ET	Daily evapotranspiration ($mm\ d^{-1}$)	-	√	-
CO_2	Atmospheric CO_2 level (ppm)	-	√	-
Soil				
SD	Soil depth (cm)	√	-	√
WCFC	Water content at field capacity (%)	√	√	√
WCWP	Water content at wilting point (%)	√	√	√
WCST	Water content at saturation (%)	√	√	√
WCAD	Water content at air dryness (%)	√	√	√
WCWET	Critical soil water content to waterlogging (%)	√	√	√
WHC	Water holding capacity (%)	√	-	√
Interactions				
SD x WS	Interaction of SD and WS	√	-	√
SD x G.WS	Interaction of SD and G.WS	√	-	√
SD x W.WS	Interaction of SD and W.WS	√	-	√
SD x Rain	Interaction of SD and Rain	√	-	√
SD x G.Rain	Interaction of SD and G.Rain	√	-	√
SD x W.Rain	Interaction of SD and W.Rain	√	-	√
WHC x WS	Interaction of WHC and WS	√	-	√
WHC x G.WS	Interaction of WHC and G.WS	√	-	√
WHC x W.WS	Interaction of WHC and W.WS	√	-	√
WHC x Rain	Interaction of WHC and Rain	√	-	√
WHC x G.Rain	Interaction of WHC and G.Rain	√	-	√
WHC x W.Rain	Interaction of WHC and W.Rain	√	-	√
T^2	Square of Tmax	√	-	√
$G.T^2$	Square of G.Tmax	√	-	√
$W.T^2$	Square of W.Tmax	√	-	√
T^2	Square of Tmin	√	-	√
$G.T^2$	Square of G.Tmin	√	-	√
$W.T^2$	Square of W.Tmin	√	-	√
10Log(Rain)	The logarithm of Rain	√	-	√
10Log(G.Rain)	The logarithm of G.Rain	√	-	√
10Log(W.Rain)	The logarithm of W.Rain	√	-	√

5.2.3 Modelling yields

Crop growth simulation model

LINTUL2 is a process-based crop growth simulation model that allows for the simulation of soft winter wheat under potential and water-limited conditions (for a comprehensive description: van Ittersum et al., 2003). LINTUL2 describes yield under water-limited conditions by including a water balance of crop and soil in the LINTUL1 model. Conditions are still optimal with respect to other growth factors, i.e. ample nutrients and a pest-, disease- and weed-free environment. The LINTUL2 model was designed to study options for water conservation, as well as differences among cultivars in drought tolerance. Input data are daily solar radiation, temperature and rainfall, plant density, dates of crop emergence and harvest; soil depth, and the soil moisture retention characteristics, i.e. the relation between volumetric soil moisture content and suction (see also Table 5-1). LINTUL2 has been used in numerous climate change studies (e.g. Wolf and van Oijen, 2002; Ewert et al., 1999).

LINTUL2 is integrated in the so-called Agricultural Production and Externalities Simulator (APES), which is a cropping system modelling framework (Adam et al., 2012). The model was further extended with various calibration methods valid for European conditions by Angulo et al. (2012) to allow the simulation of spatial and temporal yield trends and responses to climate change. Their results showed that the extended method considering the region-specific calibration of phenology and growth parameters is most suitable to simulate climate change effects on wheat yields in Western Germany (Angulo et al., 2012). This version of the model includes the effects of CO_2 levels and technology development on winter wheat yield.

Metamodel

A metamodel is considered to be the simplest parsimonious regression model that mimics the input–output relationships of the process model. A metamodel was derived from the LINTUL2 model for Western Germany. LINTUL2 was run for a ten year period (1983-1992) for the 70 climate zones for the simulation of winter wheat in Western Germany, using SPSS. This way, both spatial and temporal variability was represented in the input and output. The metamodel was obtained by relating model input to model output by means of a multiple linear regression. In this case, because our metamodel is meant to be run with coarser data than those required by the LINTUL2 model, we deliberately choose variables that are also available at wide spatial and temporal scales, i.e. soil depth in addition to the detailed variables used by LINTUL2, and annual average of daily weather data instead of daily data (see Table 5-1). Theory suggests that some variables are non-linearly related to crop yields, we included transformations (Wallach et al., 2006). For temperature, we included a squared term, to allow the regression to pick up the fact that temperature has an optimum; for precipitation we included a log transformation, to prevent that the signal from normal rain variability becomes obscured by extreme rainfall events. Furthermore, considering the fact that interactions are known to exist and may improve the results of the model, we included several interactions (see Table 5-1). The interactions were included to account for the possibility that e.g. water holding capacity becomes a more important determinant of crop yield in areas where rainfall is low. A Pearson correlation matrix was calculated to indicate the degrees of colinearity between all explanatory variables. For reasons of space, we only show those variables that were strongly related (i.e. Pearson correlation coefficient > 0.75) to at least one of the other variables. The most significant independent variables for predicting winter wheat yields were selected by means of a backward elimination of the variables with the lowest statistical significance.

Empirical model

An empirical model was created for the simulation of winter wheat in Western Germany by regressing 10 years of observed annual winter wheat yields (1983-1992) for 70 climate zones on the various predictor data in table 5-1, using SPSS. The most significant independent variables for predicting winter wheat yields were selected by means of a backward elimination of the variables with the lowest statistical significance. Because we wanted to compare the empirical model to the metamodel, both models use the same set of potentially explanatory variables. Yearly yields were considered independent events, so we did not correct for temporal autocorrelation.

5.2.4 Validation of the modelling approaches

The three model approaches were validated for a second 10 year period (1993-2002) for which also the agricultural yield statistics and predictor data were available. The results of the validation were expressed as a coefficient of determination (R^2), the root mean squared Error (RMSE), and the root mean squared Error normalized to the average of the observed values (CV-RMSE). The coefficient of determination was calculated as 1 – SSE/SST, whereby SSE is the sum of squares of residuals, and SST is the total sum of squares. The RMSE is calculated as:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(\hat{x}_i - x_i)^2}{n}} \qquad (5.1)$$

Where, $\hat{x}_i$ is the simulated yield, x_i is observed yield at climate zone *i*, and *n* is the number of observations (70 climate zones x 10 years). The CV-RMSE is calculated as $\mathrm{RMSE}/\bar{x}$, where $\bar{x}$ is the average of the observed yield.

5.2.5 Comparison of Modelling yield patterns

Different simulated regional patterns of winter wheat yields, averaged over the 10 years period (1993-2002), were compared with the observations over the same time period. The results of comparison were expressed as a R^2, the RMSE similar to Eq. (5.1), and CV-RMSE. Whereas the previous analysis (validation of the modelling approaches) is based on 700 observations, this analysis is based on 70 climate zones. This is because simulated and observed annual-yields of winter wheat yields were averaged over the 10 years period (1993-2002).

5.2.6 Simulation of future 2050 yields for Western Germany

The scenario analysis considered projected changes in temperature, precipitation, wind speed, vapour pressure, radiation, evapotranspiration, atmospheric CO_2, and technological development. The soil variables were considered constant in time. The empirical model, the LINTUL2 model, and the metamodel were used to simulate future winter wheat yield for the 20 years period centred around 2050 (2041-2061) for the climate change scenario of 15GCM A1B. We took the winter wheat yield maps for the period 1993-2002 as the baseline, and compared them with the 2050 maps to explore the predicted changes in yields.

5.3 Results and discussions

5.3.1 Crop growth simulation model

LINTUL2 outcomes explained 58% of the observed winter wheat yield variability in the validation period (1993-2002) with a RMSE of 0.73 t $ha^{-1}yr^{-1}$, and a CV-RMSE of 12%. As the model was already calibrated, we only present its performance on the validation period.

5.3.2 Metamodel

The best metamodel to emulate the winter wheat yield estimates by the LINTUL2 for the period 1983-1992 is:

$$Yield = 5.2 + 5.4\ TD + 0.2\ W.Tmin - 0.1\ G.WS$$

With:

Yield = Winter wheat yield (t $ha^{-1}yr^{-1}$)

TD = Technological development (-)

G.WS = Mean growing season wind speed (m s^{-1})

W.Tmin = Mean winter season minimum temperature (^oC)

According to this model, yields increase with increasing minimum temperature during winter, which can probably be ascribed to a reduced risk on frost damage. Yields decrease with increasing wind speed during growing season, which can probably be ascribed to the fact that winter wheat is rather vulnerable to wind damage during the growing season (Armbrust et al., 1974). Furthermore, with each unit increase in TD, yields go up with 5.4 t $ha^{-1}yr^{-1}$. As annual changes in TD fluctuate around 0.055, this comes down to an average annual increase of approximately 29 kg ha^{-1}. Soil variables were not included in the metamodel, neither were any of the non-linear or interaction terms. The metamodel predicted 72% (=R^2) of the simulated winter wheat yield variability in the validation period (1993-2002) with a RMSE of 0.45 t $ha^{-1}yr^{-1}$, and a CV-RMSE of 8%. The metamodel predicted 49% (=R^2) of the observed winter wheat yield variability in the validation period (1993-2002) with a RMSE of 0.91 $ha^{-1}yr^{-1}$, and a CV-RMSE of 15%.

5.3.3 Empirical model

The best linear multiple regression model to emulate the observed winter wheat yield for the period 1983-1992 is:

$$Yield = 13 + 6.2\ TD + 0.3\ W.Tmin - 0.2\ W.WS + 0.2\ SD$$

With:
Yield = Winter wheat yield (t $ha^{-1}yr^{-1}$)
TD = Technological development (-)
W.Tmin = Mean winter season minimum temperature (^oC)
W.WS = Mean winter season wind speed (m s^{-1})
SD = Soil depth (cm)

According to this model, yields are higher on deeper soils, which is related to rooting depth and plant available water. Furthermore, all variables are included that were also included in the metamodel, except that this model picked up wind speed during winter while the metamodel picked up wind speed during growing season. This model predicted 60% (=R^2) of the observed winter wheat yield variability in the validation period (1993-2002) with a RMSE of 0.61 t $ha^{-1}yr^{-1}$, and a CV-RMSE of 10%.

5.3.4 Spatial patterns

The observed and modelled winter wheat yield maps for 1993-2002 are presented in Figure 5-1. The observed yields, obtained at the level of administrative units, were aggregated to the 70 climate zones to allow comparison (Figure 5-1a). Figure 5-1b shows results from the empirical model, Figure 5-1c those of the LINTUL2 model, and Figure 5-1d those of the metamodel. All models have a similar order of magnitude of yield prediction and associated uncertainties. They were all capable of reproducing high-productivity regions in northern part of Western Germany as well as the low-productivity regions in southern parts. The spatial patterns and temporal trends seem to be better represented by the empirical model (R^2= 69%, RMSE= 0.49 t $ha^{-1}yr^{-1}$, and CV-RMSE= 8%) than by the LINTUL2 model (R^2= 65%, RMSE= 0.67 t $ha^{-1}yr^{-1}$, and CV-RMSE=11%) and the metamodel (R^2= 56%, RMSE= 0.79 t $ha^{-1}yr^{-1}$, and CV-RMSE=13%). This spatial variability must be associated with the spatial variability in soil depth. The absence of any soil variable in the metamodel reveals an overall insensitivity of the LINTUL2 model to soil variability. This insensitivity seems to be refuted by the spatial variability in observed crop yields. Overall, the LINTUL2 and the metamodel are able to mimic the global North-South trend, but appear not to capture the finer-scale soil variability that is visible in the empirical model and the agricultural census data. This can explain the slightly better performance of the empirical model.

5.3.5 Temporal trends

The temporal trends of winter wheat yields, observed as well as predicted by the three models, are plotted in Figure 5-2. All models simulate a general increase in average yield in time. The reported census data demonstrate a peak around 1991, which is only reproduced by the empirical model. Based on the small differences between the metamodel and the empirical model, it seems likely that this should be attributed to the higher sensitivity of the empirical model to minimum winter temperature or the fact that the empirical model used winter wind speed instead of growing season wind speed. If we plot the trend in explanatory variables – used by the metamodel and the empirical model – along with the trend in yields (Figure 5-3) it appears as if the winter wind speed was the variable that allowed the empirical model to simulate the peak in yields in 1991.

5.3.6 Simulation of future 2050 climate change effects for Western Germany

The difference of simulated future winter wheat yields (2041-2061) from the baseline yields (1993-2002) for the different modelling approaches is shown in Figure 5-4. Projected future yields were higher than baseline yields for all modelling approaches, although the increase varied considerably per geographical area. Yield increases were highest for the empirical model, showing an increase in yields between 1% and 60% (on average 19%). The metamodel predicts a yield increase between 3% and 56% (on average 18%). It shows a more modest change in the yields but still with considerable increases in the south eastern part of the region. The LINTUL2 model predicts the smallest yield increase, between 5% and 44% (on average 17%). Overall future increases in winter wheat yield (Figure 5-2 and Figure 5-4) can obviously be ascribed to technological development, and for the LINTUL2 projection also to elevated atmospheric CO_2. It is remarkable that both the metamodel and the empirical model predict higher future yields than the LINTUL2 model, in spite of not being sensitive to increased CO_2 levels. This could indicate a structural overestimation of a positive effect of one of the other variables, such as winter temperature or technological development. It also may indicate that such positive effects are highly correlated with elevated CO_2. The spatial variability in the metamodel and the empirical model outcomes suggests that changes in yield are also determined by variables exhibiting, next to temporal variability, also spatial variability. These are winter temperature, and wind speed. Particularly, consideration of technology development can have substantial impacts on yield prediction. Further investigation is required to reduce uncertainty in the assumptions regarding technology development, especially for future projections of crop yields within climate scenarios.

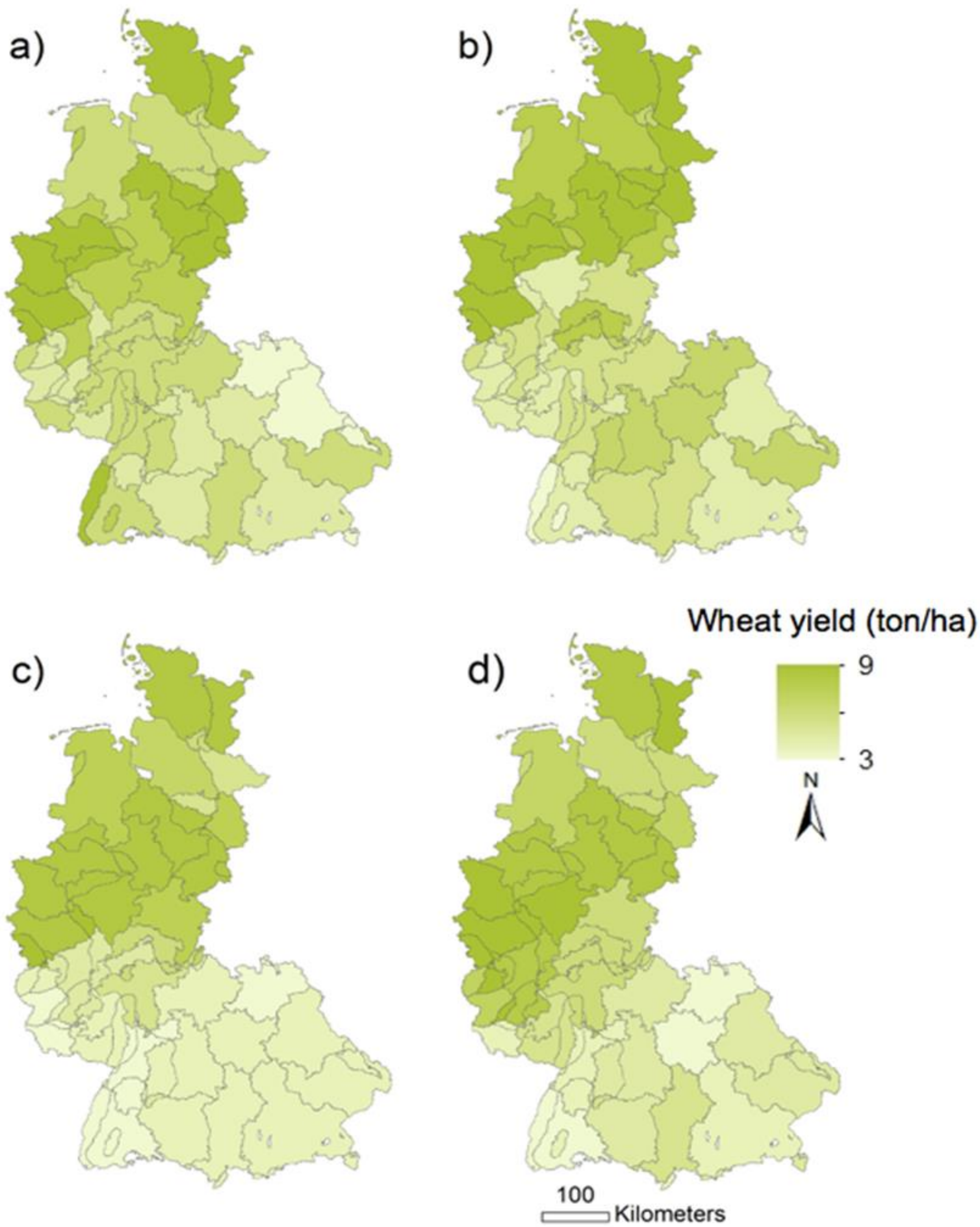


Figure 5-1: Winter wheat yields averaged over the period 1993-2002, showing yields per climate zone region based on: a) agricultural statistics, b) empirical model, c) LINTUL2, and d) metamodel.

Table 5-2: Pearson correlation coefficient between variables in the empirical and metamodel approach (Only variables with one or more correlations stronger than 0.75 are shown)

	WCFC	WCST	WCWP	Rain	TMax	TMin	SRAD	WS	ET	VP	W. Tmax	W. TMin	W. WS	G. Tmax	G. TMin	G. SRAD
WCST	0.75	1														
WCWP	0.83	0.98	1													
WCWET	0.94	0.93	0.96													
TMin	-0.07	-0.10	-0.10	0.14	0.79	1										
ET	0.08	0.08	0.08	-0.22	0.78	0.30	0.85	-0.27	1							
VP	-0.06	-0.08	-0.08	0.16	0.79	0.99	-0.01	0.17	0.31	1						
W.Tmax	-0.06	-0.08	-0.09	-0.13	0.90	0.78	0.32	-0.01	0.61	0.75	1					
W.TMin	-0.06	-0.11	-0.10	0.00	0.82	0.93	0.10	0.13	0.40	0.88	0.91	1				
W.WS	-0.11	-0.14	-0.15	0.15	-0.01	0.31	-0.44	0.96	-0.15	0.30	0.08	0.26	1			
W.VP	-0.08	-0.12	-0.12	-0.01	0.82	0.93	0.06	0.14	0.37	0.89	0.91	0.99	0.26			
G.Rain	0.05	0.10	0.10	0.86	-0.27	-0.14	-0.03	-0.05	-0.14	-0.10	-0.32	-0.28	-0.07			
G.Tmax	0.02	0.01	0.01	-0.14	0.90	0.63	0.49	-0.21	0.79	0.66	0.66	0.61	-0.04	1		
G.TMin	0.01	0.01	0.02	0.23	0.74	0.87	0.12	0.14	0.44	0.91	0.61	0.72	0.28	0.76	1	
G.SRAD	0.10	0.10	0.11	-0.37	0.54	0.21	0.86	-0.34	0.84	0.20	0.48	0.37	-0.20	0.61	0.24	1
G.WS	-0.16	-0.15	-0.16	0.12	-0.23	0.08	-0.54	0.97	-0.35	0.08	-0.10	0.01	0.69	-0.32	0.03	-0.42
G.ET	0.08	0.07	0.07	-0.25	0.76	0.37	0.77	-0.26	0.94	0.37	0.56	0.45	-0.08	0.86	0.50	0.90
G.VP	0.02	0.02	0.03	0.19	0.76	0.87	0.15	0.14	0.47	0.91	0.64	0.72	0.29	0.77	0.99	0.27

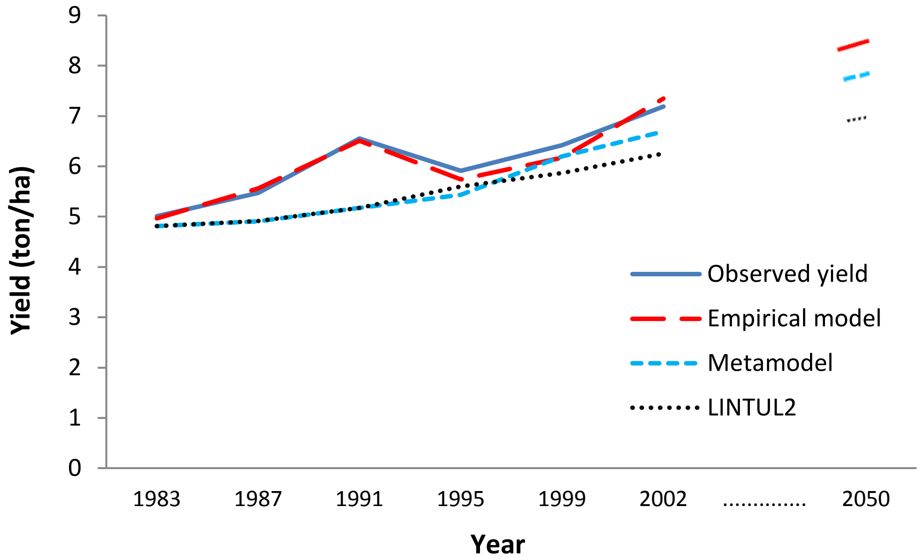


Figure 5-2: The temporal trend of observed and simulated winter wheat yields from 1983 to 2050 for Western Germany.

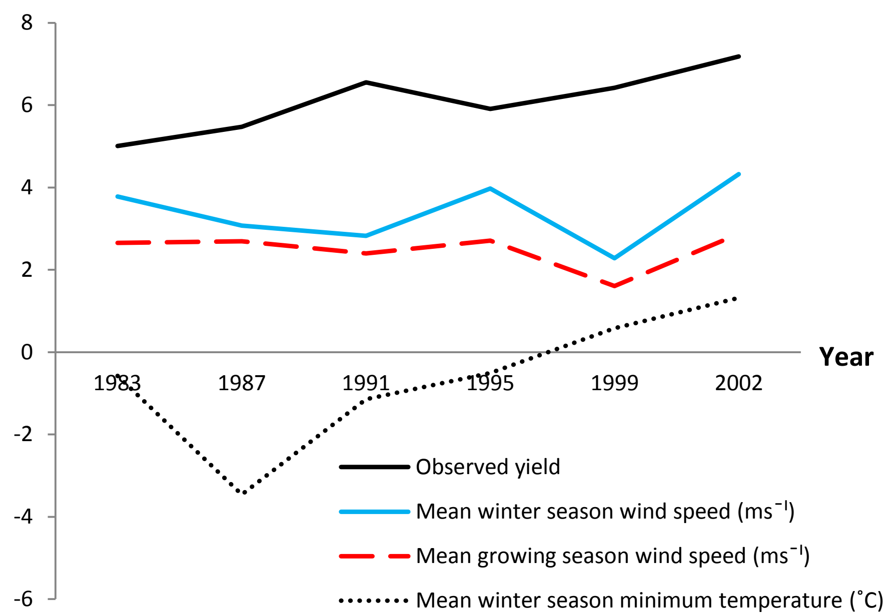


Figure 5-3: The difference between wheat yields in 1993-2002 and 2041-2061, simulated by: a) empirical model, b) LINTUL2, and c) metamodel.

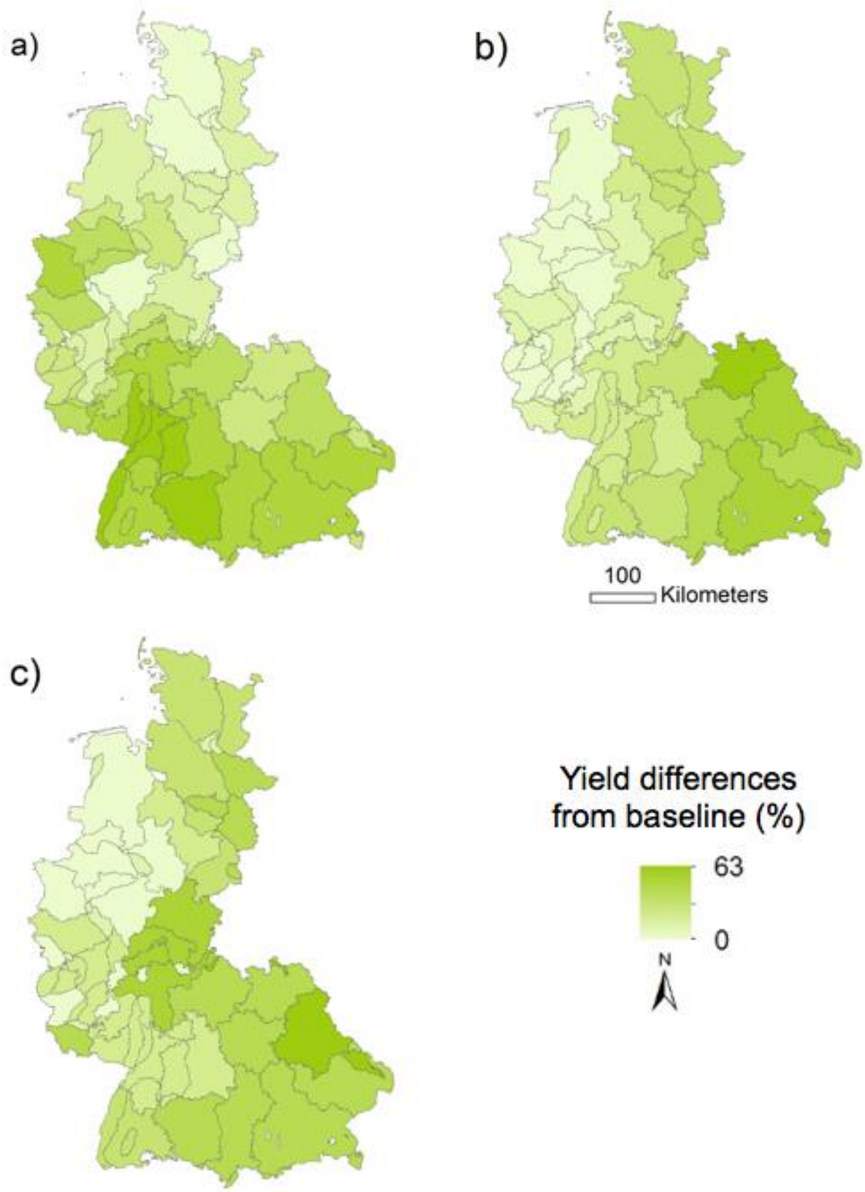


Figure 5-4: The temporal trend of variables included in metamodel and empirical model from 1983 to 2002 for Western Germany.

5.3.7 Model comparison

We compared different modelling approaches in order to simulate and predict crop yields at wide spatial and temporal scales. Apart from the inherent differences of the proposed models all three seem reasonably able to predict winter wheat yield level at regional to national scales. The fact that all approaches have similar model performances could be somewhat overestimated due to aggregation effects of reported yields. The yields were aggregated either by administrative units (Figure 5-1) or for the whole of Western Germany (Figure 5-2). It is known from landscape scale studies that such aggregation steps can cause a scale-dependent overestimation of model fits (Veldkamp et al., 2001). Whether this effect has caused some overestimations of model performance or not, does not matter in the sense that it affected all three models in a similar fashion.

A model comparison helps to reveal shortcomings and strengths of the models. For example: in our study, a performance comparison between the three models indicated that a higher sensitivity to soil depth in the LINTUL2 model and the metamodel would probably lead to better predictions of yield spatial variability. Moreover, a performance comparison between the three models indicated that a higher sensitivity to winter wind speed in the LINTUL2 model and the metamodel would probably lead to better predictions of yield temporal variability. The best fit with reported reality is observed for the empirical model, apparently outperforming the crop growth simulation model and its derived metamodel.

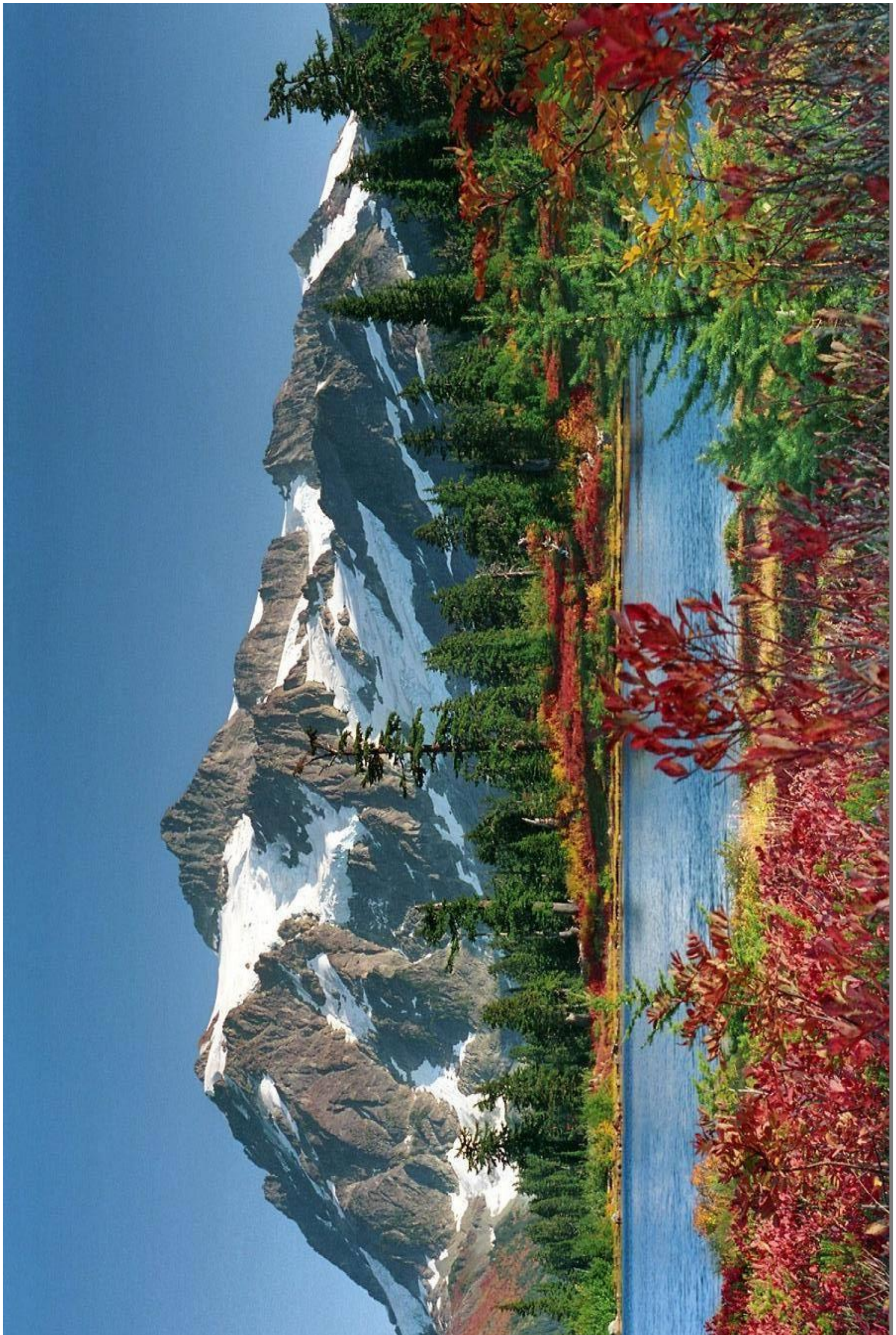
However, the fundamental limitation of the empirical model is that it is not valid outside its calibration domain severely hampers its usefulness for future predictions (White, 2009). Their validity for long-term future projections, especially that of empirical models that are calibrated on past observations, is however questionable. Future projections of crop yields within climate change scenarios can be best made by crop growth simulation models. The added value of the metamodel is that it is much faster to run and it requires far less data as the original LINTUL2 model. This suggests that such metamodels could be successfully used for fast, quick scan applications of future yield scenarios for areas where LINTUL2 has been calibrated. The empirical models and the metamodels are easy to make, require less input variables compared to the CGSMs to estimate regional patterns of crop yield. For Western Germany, the metamodel and the empirical model required three and four input variables respectively, while the CGSM required 16 input variables. The strength of empirical models and metamodels is that for their application they only require input data for variables that are selected to be relevant for the region or crop of interest (Lobell and Burke, 2010; Landau et al., 2000).

Remarkable is furthermore that neither the empirical model nor the metamodel contain a precipitation variable. Rainfall was also not strongly correlated to any of the variables that were included, which would account for its absence. Apparently, in the study area and during the study period, neither spatial nor temporal variability in rainfall was strongly related to either modelled or observed yields.

All three models are limited by the fact that they assume that other mainly socio-economic factors do not directly drive crop productivity. This could be easily overcome by using such data to derive improved empirical models. The general validity of such simplistic models is questionable because many mechanisms of the complex multi-level land system are still unknown (Veldkamp, 2009). In order to do this properly far more advanced statistical analyses are required (Bakker and Veldkamp, 2012) and the derived 'models' have no future predictive power.

5.4 Conclusions

All three explored model options have the capability to simulate and predict crop yields at wide spatial and temporal scales. The suitability of the three models used are context dependent. For near-future projections, the empirical model appeared to be most reliable. We know, however, that it is not sensitive to variables or non-linearities that will probably become important in the future. For that reason, future projections of crop yields within climate change scenarios can be best made by crop growth simulation models. The derived metamodels can be fast and reliable alternatives for areas with well calibrated crop growth simulation models. A model comparison helps to reveal shortcomings and strengths of the models. In our case, a performance comparison between the three models indicated that a higher sensitivity to soil depth and winter wind speed in the LINTUL2 model and the metamodel would probably lead to better predictions. This specific conclusion is only valid for winter wheat growth in western Germany, for the used models.



6 General discussion and synthesis

6.1 Introduction

This thesis aimed to develop a framework for recommendable practices to model regional patterns of crop yield. The sub-objectives were:

- To provide decision rules for selecting appropriate approaches to generate input variables to feed crop growth simulation models at the regional level;
- To provide decision rules for selecting appropriate procedures to simulate regional yield patterns using CGSMs;
- To identify, given context conditions, the most suitable modelling approach to simulate regional patterns of crop yield.

In this chapter, I will discuss the outcomes of these objectives. I will first summarize the main findings of the previous chapters, in the context of the above sub-objectives; then I will synthesize the findings in order to address the main objective: the framework for recommendable practices to model regional patterns of crop yield.

6.2 Accomplishment of the specific research objectives

6.2.1 Generating input at the regional level

Crop growth simulation models (CGSMs) require extensive input data on cultivar, management, weather, and soil conditions that are unavailable in many parts of the world. The validity of CGSM predictions over a region depends on the quality of the representation of the spatial variability of the input data (Hansen and Jones, 2000). At the regional scale, data availability often limits the generation of spatially detailed input data required by many CGSMs (Carbone et al., 2003). There are many approaches available to generate spatial variability in input data for CGSMs at the regional level, although criteria for the selection of the methods are often unclear. Chapter 2 discussed the issue of input data availability, and reviewed literature for existing approaches that have been used to overcome the problem of data availability. Based on the review decision rules were formulated as to what approach to take under different circumstances. Which of the approaches should be used depends on a number of questions whose answers lead to the decision rules denoted in Figure 6-1.

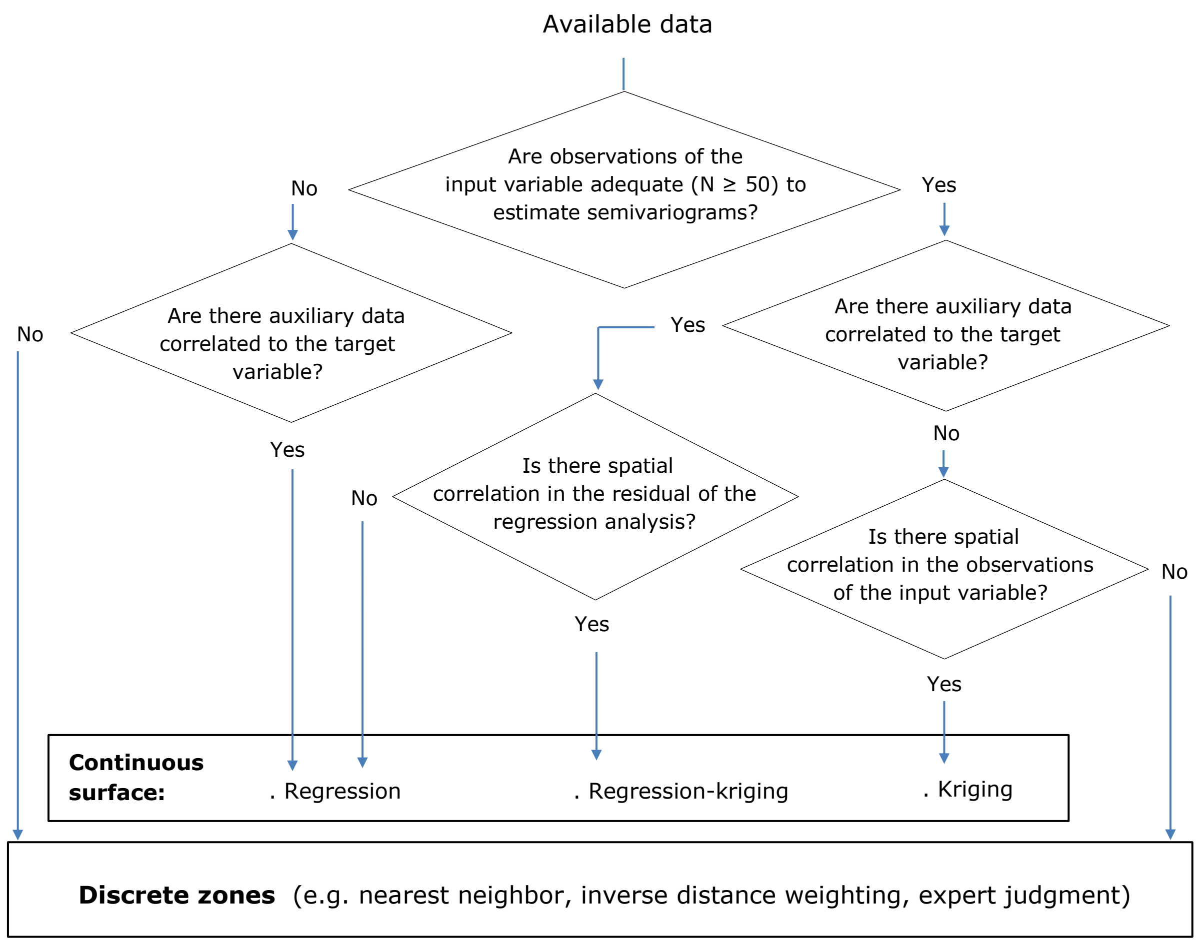


Figure 6-1: Decision rules for selecting appropriate approaches to describe the spatial variability of input variables to feed crop growth simulation models at the regional level (scale effects not included).

For quite a while, the use of discrete zones and limited use of auxiliary data has been quite common to describe the variability in weather, soil, and management. However, increasingly the input data are presented as continuous surfaces. This has the following reasons: (i) the surge of available auxiliary data such as DEMs; (ii) the accumulation of data sources (in digital form); and (iii) the development of interpolation techniques that effectively uses auxiliary data. For example, interpolation may be supported through the use of spatially referenced environmental data layers such as the global 90-m resolution DEM from the Shuttle Radar Topography Mission (Jarvis et al., 2008). Moreover, remote sensing data can be considered as auxiliary data to use in the interpolation of soil and weather data.

Currently, with improved tools like geographical information systems (GIS) and field computers, more point data are saved during soil surveys than before. Moreover, because soil data do not change much over time, observations typically accumulate over time. The increased availability of soil observations allows for moving from discrete zones to continuous surfaces by means of interpolation.

An advanced form of interpolation, where the use of auxiliary data is formalized, is digital soil mapping (DSM) (see e.g. Kempen et al., 2011). Recently, few studies have combined general pedological knowledge with interpolation methods to map the three-dimensional variation of soil properties using depth functions (Kempen et al., 2011; Malone et al., 2009; Meersmans et al., 2009; Mishra et al., 2009). Some weather, soil, and management variables can also be observed continuously, for example, by satellites (e.g. Launay, 2002; Guerif and Duke, 2000; Hansen and Jones, 2000). The big advantage of these measurements is that they directly result in continuous (small pixels) surfaces of variables. However, direct observation of soil properties by satellites is limited to topsoil, and only for cases where the soil is bare and not too many clouds occur. Interestingly enough there is very little use of mechanistic models to create continuous surface of weather data (e.g. Baigorria, 2005) and soil data (e.g. Finke, 2012; Minasny and McBratney, 2001) to feed CGSMs. Clearly, more research is needed to create continuous surface of management data by mechanistic models to feed CGSMs at the regional level.

Generally, spatially-explicit regional patterns of yield are less accurate when done for discrete zones compared to continuous surfaces, although one should be aware of a false sense of accuracy, when continuous maps are made by unreliable interpolations. The most suitable method should be selected in a structural way, using decision rules as presented in Figure 6-1, rather than to limit ourselves in an early stage to the typical procedures such as discrete zones.

6.2.2 Procedures for using CGSMs at the regional scale

Regional patterns of crop yields using CGSMs can be generated with two different approaches: (i) run the CGSM for a series of points distributed throughout a region after which the simulated crop productions can be interpolated to create a continuous surface of yield patterns (calculate first, interpolate later; CI), and (ii) create surfaces for each of the input variables individually, then run the CGSM for each location (grid cell) to create a continuous surface of yield patterns (interpolate first, calculate later; IC). In order to generate reliable model results for regional applications and/or estimate associated uncertainties, it is important to understand and consider the influence of the sequence of model calculations and interpolations (i.e. CI and IC) on simulation results, especially in the case of complex models with non-linear relationships (Ewert, 2004).

I evaluated and compared these two approaches, by applying SUBSTOR-potato model (Ritchie et al., 1995) for potato to the Carchi province in Northern Ecuador at different supports, as illustrated in Figure 3-2 in Chapter 3. By using different supports, I examined scaling effects that arise from spatial variability in soil properties. The interpolations were performed with kriging at 100 m resolution. The specific objective was (i) to find the influence of the sequence of model calculations and interpolations (i.e. CI and IC) on the prediction of spatial patterns of potato yield, and (ii) to evaluate the persistence of the CI and IC results with different supports, both spatially and non-spatially. Model performance was compared with interpolated, observed yields at resolutions of 100 m and 400 m.

In theory the two approaches are expected to produce the different results when the CGSM and / or interpolation method are nonlinear (Groot et al., 1998; Heuvelink, 1998; Addiscott and Tuck, 1996; Addiscott, 1993). It can be expected that the deviation is proportional to the degree of non-linearity of the model or interpolation method (Addiscott and Tuck, 2001). Moreover, there are other factors, including the spatial dependency of input variables and the correlations between the input variables, which can contribute to the difference between the results of the CI and IC approach (see e.g. Van Bodegom et al., 2002; Addiscott and Tuck, 2001; Heuvelink and Pebesma, 1999). Anticipating how these factors' interactions will affect the differences between the two approaches is difficult. Therefore, in this thesis (Chapter 3) I took an experimental approach to understand and consider the role of these different factors in the differences between the two approaches.

This study revealed a clear difference between the CI and IC approach. In the Carchi region, where this study was conducted, all soil properties were characterized by a nugget-to-sill ratio less than 41%, and a (autocorrelation) range of about 3.5 km. The individual inputs (i.e. soil properties in this case) showed different spatial dependency. Although these differences were small, they can explain the difference between the results of the CI and IC approach. This is because interpolation of the individual inputs can take these differences into account whereas spatial interpolation of the output cannot (see e.g. Heuvelink and Pebesma, 1999). On the other hand, the output of the CGSM had an even larger range than the ranges of soil properties. This is partly due to the model non-linearity, as interaction of model non-linearity with the spatial dependency of inputs increases the range in the CI approach (Leterme et al., 2007).

In general, with interpolation and / or aggregation variability of data will decrease and local extremes will be levelled out (Baron et al., 2005; Bodegom et al., 2002; Bouma et al., 1996). Depending on the spatial distribution, this effect will be stronger for some variables than for others. As a result, correlations between variables may change with interpolation and / or aggregation. Such changes may be a cause of difference between the results of the CI and IC approaches (Van Bodegom et al., 2002; Heuvelink and Pebesma, 1999). In order to see to what extent this has been the cause for the difference between the IC and the CI approach, three Pearson correlation matrices were calculated to indicate the degree of colinearity between all soil properties at point level, at 100 and at 400 m resolutions. The matrix calculated at point level shows that some of soil properties are strongly correlated. However, in this case study, the data correlation between all soil properties did not change from point level to 100 m, nor did it change from point level to 400 m resolution.

Final results demonstrate that the order of calculation and interpolation was of major importance, while aggregation had a minor effect on the regional patterns of potato yield in the Carchi study area. The former is probability due to the non-linearity of CGSM and the difference in the spatial dependency of individual inputs; the latter is probably due to the absence of local extremes, which is due to the gradual trends in soil properties in the volcanic ash soils of Carchi (being a result of the soil forming processes, but also a consequence of the interpolation method, kriging). The RMSD in the normalized yields was 0.79 for the CI approach and 0.99 for the IC approach at 100 m. For the aggregation to 400 m, the RMSD was 0.74 for the CI approach and 0.99 for the IC approach. The spatial comparison of regional patterns of crop yield in terms of the semivariogram parameters (i.e. nugget-to-sill ratio and range), the Moran’s I (Li et al., 2007; Moran, 1950), and visually, shows that regional yield patterns generated by different procedures (i.e. different approaches and different supports) were similar, while, non-spatial comparisons of different yield patters in terms of RMSD showed better performance of the CI approach than the IC approach. From an uncertainty propagation and variability point of view it is in general preferable to calculate first before interpolation.

6.2.3 Modelling-approach comparison

Models are typically evaluated in terms of their credibility in modelling yield patterns, on the basis of a range of observation points using statistical techniques like the root mean square difference (Akinbile and Yusoff, 2011; Quiroga and Iglesias, 2009; Xiong et al., 2008). Since there will always be a certain level of idiosyncrasy to the case, one has to strive for a toolbox of approaches from which the proper tool can be selected on the basis of a number of specific criteria such as credibility, sensitivity, and user friendliness that are defined in this thesis.

Credibility

I evaluated the performance of three different models for their capacity to predict regional patterns of crop yield for two different regions: the Carchi province in Northern Ecuador and Western Germany. In the Carchi area, the model evaluation was done on the basis of a large farm survey in a relatively small but heterogeneous mountain area. In Western Germany, a similar evaluation was done, but based on census data and for larger climate zones. For the Carchi study area, spatial analyses were carried out at watershed level, while for Western Germany spatial and temporal analyses were carried out at national level. The CGSM used for the Carchi study area was the SUBSTOR-potato model (Ritchie et al., 1995) that was calibrated and validated for Andean conditions using experimental data from the region (Bowen et al., 1999; Clavijo, 1999) (for a comprehensive description see Annex); the CGSM used for Western Germany was the LINTUL2 model (van Ittersum et al., 2003) that was - to some extent - adapted to wider spatial and temporal scales: it includes a technology development factor and it was recalibrated for spatially aggregated input data (Angulo et al., 2012) (for a comprehensive description see Annex).

In both case studies the metamodels were obtained by relating model input variables to simulated crop yield by means of a multiple linear regression. The existence of a validated CGSM is the most important requirement for the metamodel approach. In both case studies the empirical models were obtained by relating various explanatory variables to observed crop yield by means of a multiple linear regression. For the empirical models and metamodels, the most significant explanatory variables for predicting crop yields were selected by means of a backward elimination of the variables with the lowest statistical significance.

For the Carchi study area, the maps of the different modelling exercises all demonstrated a good correspondence with the map of observed yield, evaluated visually and in terms of RMSD. The different modelling approaches properly identified the high-productivity regions in the western part, where altitudes are between 3000 and 3300 m.a.s.l., as well as the low-productivity regions (Figure 4-2, Chapter 4). The RMSD values for the difference between the three model-based maps and the map of observed potato yields show that the differences were lowest for the empirical model, with a RMSD of 0.61. The RMSD was highest for the metamodel, with a RMSD of 1.05. The CGSM showed a RMSD of 0.99. The empirical model outperformed the CGSM and the metamodel in being better able to capture the regional pattern of potato yield. This might be explained by causes such as pest and diseases, which are not represented in the CGSM nor in the metamodel.

In Western Germany, all models have a similar order of magnitude of yield prediction and associated uncertainties. They were all capable of reproducing high-productivity regions in the northern part of Western Germany as well as the low-productivity regions in southern parts. The spatial patterns and temporal trends seem to be better represented by the empirical model (R^2= 69%, RMSE= 0.49 t $ha^{-1}yr^{-1}$, and CV-RMSE= 8%) than by the LINTUL2 model (R^2= 65%, RMSE= 0.67 t $ha^{-1}yr^{-1}$, and CV-RMSE=11%) and the metamodel (R^2= 56%, RMSE= 0.79 t $ha^{-1}yr^{-1}$, and CV-RMSE=13%). This spatial variability must be associated with the spatial variability in soil depth. The absence of any soil variable in the metamodel reveals an overall insensitivity of the LINTUL2 model to soil variability to simulate winter wheat growth in this specific case study. This insensitivity seems to be refuted by the spatial variability in observed crop yields. Overall, the LINTUL2 and the metamodel are able to mimic the global North-South trend, but appear not to capture the finer-scale soil variability that is visible in the empirical model and the agricultural census data. This can explain the slightly better performance of the empirical model.

Moreover, Chapter 4 analyses the effect of spatial aggregation on the performance of the modelling approaches with the aim of analysing models' relevance by modelling the yield patterns at support resolutions larger than field. In the Carchi study area, all yield maps (observed and model-based) were aggregated to higher aggregation levels of 200, 300, 400, 500 and 600 m resolutions. Subsequently, the model-based yield maps were compared to the interpolated, observed yields in terms of Root Mean Squared Difference (RMSD). In this study, the rates of decreasing RMSD with higher aggregation levels were similar for the different modelling approaches and in most cases resulting in a linear decline of 15-30%. The results showed that aggregation of calculated data leads to less variability and increasing linear fits at higher aggregation levels. The spatial variability in the case study area determines how strong this effect is.

To conclude, all three modelling approaches were capable to predict the observed regional patterns of crop yield in both case studies and are therefore considered to be credible. However, in both case studies the empirical models outperformed CGSMs in being better able to simulate the regional patterns of yield. The metamodels were also able to simulate regional patterns of crop yields, albeit always less accurate than the CGSMs.

Sensitivity

I compare the models in terms of the models' sensitivity to the different explanatory variables and the models' application domain.

Explanatory variables

From the results of Chapter 4 (i.e. the Carchi case study), it can be observed that the empirical model and metamodel exhibit a sensitivity to soil water holding capacity and weather variables, as these were important explanatory variables. The sensitivity of all three modelling approaches to weather variables and water holding capacity suggest that the potato yield in the Carchi study area is driven by temperature and constrained by water availability. From the results of Chapter 5 (for Western Germany), it can be observed that the metamodel exhibits a sensitivity of the original CGSM to technological development, wind speed, and minimum winter temperature. The empirical model demonstrated, in addition to technological development and weather variables a further sensitivity of the actual yields to soil depth. The weather variables included in the metamodel and the empirical model were largely the same, except that the empirical model picked up wind speed during winter while the metamodel picked up wind speed during growing season.

Based on results of Chapter 5 (i.e. the Western Germany case study), I could derive that the LINTUL2 model appeared to lack sensitivity to wind speed during winter to adequately model temporal variability of winter wheat yields in this specific case study. Because the sensitivity of the empirical model to winter wind speed resulted in a better performance of this model, the empirical model could be used to reveal these shortcomings of the process-based model. Moreover, LINTUL2 appeared to lack sensitivity to soil variables to adequately model spatial variability of winter wheat yields in this specific case study. The fact that the empirical model was able to predict spatial variability in observed data, suggests that the

LINTUL2 model would probably benefit by a higher sensitivity to soil variables as well as wind speed during winter. This specific conclusion is only valid for winter wheat growth in western Germany, for the used models.

To conclude, regional patterns of crop yield are determined by a limited number of explanatory variables. The importance of the various explanatory variables in the empirical model and metamodel in response to yield is obvious and can be derived from their statistical significance. In the case of CGSMs, a sensitivity analysis is required to derive the importance of the various explanatory variables in response to yield. The development of a metamodel could be a good alternative for the sensitivity analysis to show the importance of the various explanatory variables in the CGSMs. This is because the metamodel is constructed by identifying the most significant explanatory variables of the calibrated CGSM in response to crop yield, for a particular setting (in time and space).

Application domain

In Chapter 4 (Carchi case study) and 5 (Western Germany case study) the empirical model and metamodel demonstrated a sensitivity to weather variables. Therefore, the weather variables in the empirical and metamodel allow for their potential use in climate change scenarios. However, their validity is probability limited to near-future predictions. Empirical models and metamodels can be used if the range of the input variables for the simulation does not exceed the range of the input variables in the calibration dataset by, say, more than 10% (this percentage can be made a function of the sensitivity of the model to the variable). This seriously hampers their usefulness for scenario studies (White, 2009). For the prediction of future patterns or for wider agro-ecological conditions both the metamodel and the empirical model have fundamental shortcomings, as they may have omitted variables that are important process variables. CGSMs do take into account many factors in a way that would not be possible using empirical models and metamodels (Lobell and Burke, 2010; Bouman et al., 1998). Therefore, empirical models and metamodels are context dependent (both spatially and temporally) and should not be used for situations that deviate strongly from this context (Bakker and Veldkamp, 2012).

User friendliness

This criterion is only relevant if the developed model is to be run by non-experts (i.e. often policymakers). I considered three model characteristics to compare the user-friendliness: the number of input variables required, computation time, and transparency.

The empirical models and the metamodels require less input variables compared to the CGSMs to estimate regional patterns of crop yield (Chapters 4 and 5). The strength of empirical models and metamodels is that for their application they only require input data for variables that are selected to be relevant for the region or crop of interest (Lobell and Burke, 2010; Landau et al., 2000). As regional scale often imply that the availability of input data decreases, a limited number of input variables required by the simpler models (e.g. empirical models and metamodels) is a useful characteristic to look at for focusing further data collection on these variables.

For large-scale applications in which a lot of model runs would be required, comparison of the relative computation time under the same conditions (i.e. CPU, memory and software) may provide useful information for choosing a more efficient modelling approach (Guo et al., 2010). In both case studies (Chapters 4 and 5) the empirical model and the metamodel prove to be relatively simple and fast (= 45 second), while the CGSM required more computation time (= 600 second). The results were in agreement with the conclusions of Blanning (1975) who proposed the use of simplified models such as metamodels to obtain useful sensitivity information with a significant reduction in the computation time.

All three modelling approaches require significant expert knowledge for their development and calibration. However, after this initial phase, the empirical model and the metamodel are simple and transparent. The CGSM is a more complex model that is less transparent for non-experts and acts like a black box for non-expert users. Therefore, when the model itself is to be run by policymakers, empirical models and metamodels may be a better choice.

6.3 Synthesis

I propose a standard protocol for guiding and justifying model- and data-selection procedures for the simulation of regional yield patterns. This has led towards the design of a framework for recommendable practices to model regional patterns of crop yield, which is shown in Figure 6-2. Such a framework requires the development of general decision rules - associated with specific conditions - that will help researchers and policymakers to select model and data generation procedures that fit their objective. Although two case studies may not be enough to derive generally valid decision rules, the findings and experiences gained during the writing of this thesis certainly provide some direction towards the design of the framework for recommendable practices to model regional patterns of crop yield.

The framework consists of three elements: (i) the modelling-approach choice, (ii) the data-handling choice, and (iii) the model-implementation choice, discussed in the following.

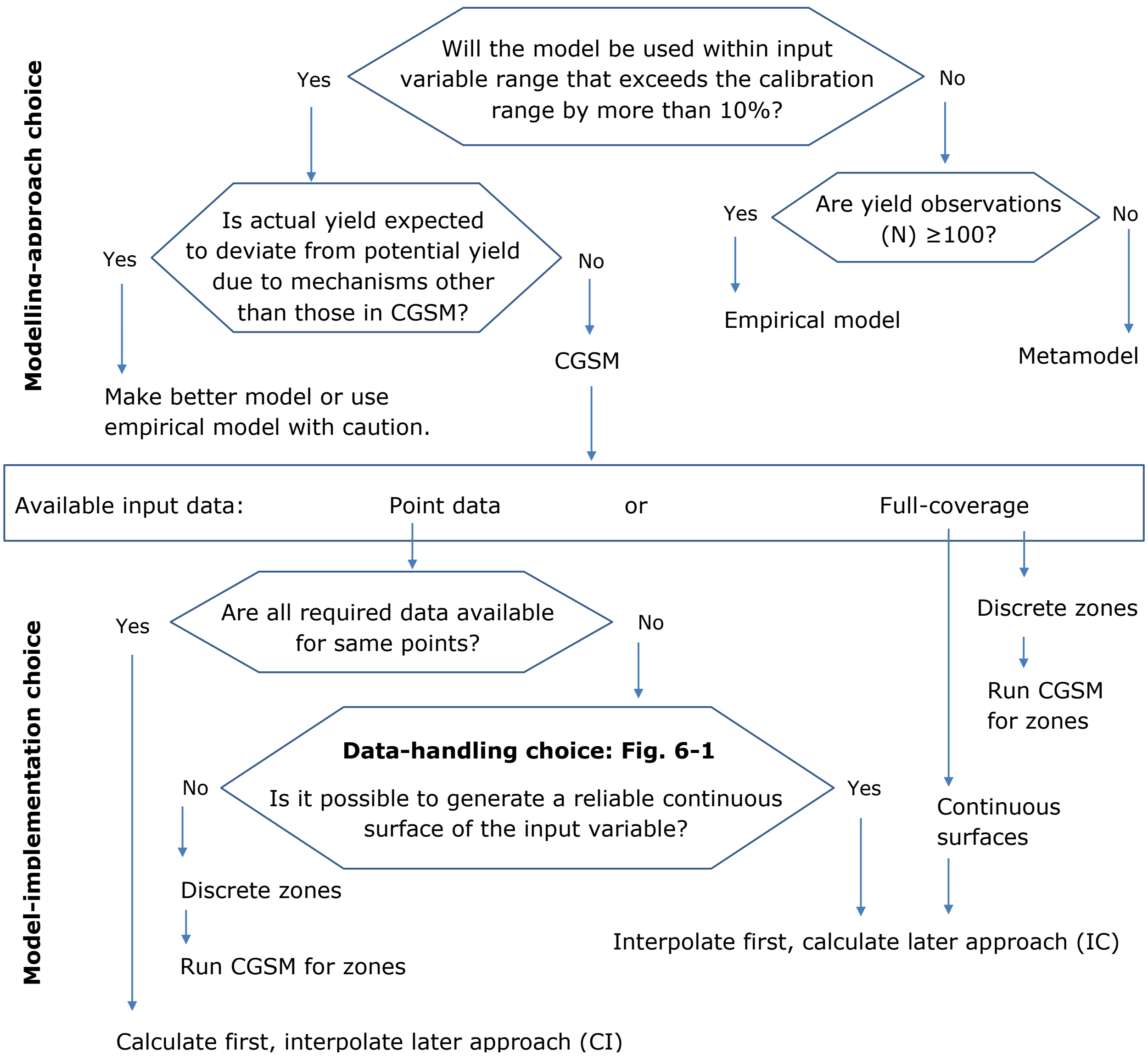


Figure 6-2: A framework for recommendable practices to model regional patterns of crop yield. The framework is context specific and not case proof.

The modelling-approach choice

Three different modelling approaches, being empirical models, CGSMs, and metamodels of the CGSMs, were distinguished to simulate regional patterns of crop yield. The context conditions that determine the best approach are input data requirements, problem definition, study sub-objective, the scale at which output results are expected, model end-users, and utilization of the output (e.g. testing different scenarios). Which of these modelling-approaches should be used depends on a number of questions whose answers lead to the decision rules denoted in Figure 2-2.

Will the model be used within input variable range that exceeds the calibration range by more than 10%?

- Empirical models can be used if the range of the input variables for the simulation does not exceed the range of the input variables in the calibration dataset by, say, more than 10% (this percentage can be made a function of the sensitivity of the model to the variable).
- When a variable does not exhibit variability within the area or time period considered, will not be included in the empirical or metamodel made for that area and time period. This does not mean that the variable is not an important explanatory variable of crop yield. CGSMs do take into account many factors in a way that would not be possible using empirical models and metamodels. The empirical models rely on existing data and are not able to make future projections of yields, when the range in input data for the future scenarios strongly exceeds the calibration range. Therefore, empirical models and metamodels are context dependent (both spatially and temporally) and should not be used for situations that deviate strongly from this context.
- For creating maps of past and current yields an empirical model will give the best results; for future scenarios, or for understanding the role of a particular variable, CGSMs should be used. Or when necessary e.g. used by or with non-experts, metamodels made from CGSMs should be used.
- When there is abundance of data, it is always recommendable to use a process-based CGSM. Due to data limitations and scale-effects, running a CGSM is often impossible. Policy makers then have to choose for either a metamodel or an empirical model.
- Empirical models are good at mimicking patterns, but due to confounding issues, the exact role of individual variables is not accurately assessed. For that reason, if one wants to

investigate the response to a change in one particular variable (e.g. temperature), it may be better to use a metamodel.

Is actual yield expected to deviate from potential yield due to mechanisms other than those in CGSM?

- Risk-factors such as pest and plagues are not captured in CGSMs. If, in general, actual yields strongly differ from potential yields for other reasons than mechanisms modelled in the CGSM, an empirical model should be considered (possibly in addition to the CGSM).

Are yield observations (N) ≥ 100?

- Creating a reliable empirical model requires a sufficient number of observations of the target variable (yield). For calibrating a CGSM less such observations are required, because calibration here concerns adjusting priorly-defined relationships rather than establishing relationships purely from the data. Calibrating a metamodel only requires a calibrated CGSM.

The model-implementation choice

With respect to model implementation, the available input data determine the possible approaches to simulate regional patterns of crop yield using field-level CGSMs. As a starting point, it is important to know whether the input data are available for a series of points distributed throughout a region. In the case of point data, two possible approaches exist (i.e. calculate first, interpolate later: CI, and interpolate first, compute later: IC) to create a continuous surface representing the spatial patterns of crop yield. Which of these approaches should be used depends on a number of questions whose answers lead to the decision rules denoted in Figure 2-2. Otherwise, (i) in the case of discrete zones describing the variability in input data, the simulations are only done for individual discrete zones resulting in a map with discrete zones characterized by the resulting simulated crop yield. In some cases (e.g. the Western Germany application), important variables are already in the form of discrete zones, and the underlying observations from which these zones were made are not available. In that case one has no option but to use the discrete zones approach. (ii)

In some cases, important variables are already in the form of continuous surfaces (e.g. remote sensing imagery). In that case one has no option, the simulations are only done for individual cells resulting in a map with continuous surfaces characterized by the resulting simulated crop yield.

Are all required data available for same points?

• If data of different input variables is collected for the same point locations, using the calculate first, interpolate later approach is best. Note however, that application of the field-level model at a larger support could have implications for model outcomes. If the latter is expected to be important, because the model is strongly non-linear, or because variables are multiplied in the model while showing strong correlation in reality, the aggregation step should be applied after model calculation.

Is it possible to generate a reliable continuous surface of the input variable?

• If data of different input variables are not collected for the same point locations, but the input variable shows good correlations with available auxiliary data, interpolation will probably results in reliable maps (see the data-handling choice), so that one can best use the interpolate first, calculate later approach. Note however, that with a complex model, applying the interpolate first, calculate later approach requires a relative high computation time, as the model needs to be run for each individual pixel to create a continuous surface of yield patterns. If the computation time is expected to be a limiting factor, an empirical model or metamodel should be considered.

• When the input data are available for only a limited number of observations, the use of discrete zones representing specific combinations of soil, weather and management data is recommended (see the data-handling choice). Representing the outcome in such zones avoids a false impression of accuracy. In case a continuous surface was created with just as poor a quality as the discrete zones, users could mistake the continuous surface output for being more realistic and accurate.

The data-handling choice

Various choices for generating data to feed CGSMs at the regional level were distinguished, based on data availability, the spatial and temporal variability of the data, the correlation with other variables, the data acquisition methods, the expected accuracy from a particular approach used to describe spatial variability, and the sensitivity of the CGSM to the variable. To structure the review of approaches that have been used in the literature, I distinguished between two categories: (i) where input data are generated as discrete zones; and (ii) where input data are generated as continuous surfaces. Obviously, the latter approach is more sophisticated, and likely to result in more accurate spatially-explicit yield predictions. However, in order to generate continuous surfaces, a few conditions need to be met, which are outlined in the decision tree in Figure 6-1.

6.4 Conclusions

The final conclusions of the research presented in this thesis are:

- Regional crop yield modelling is very sensitive to the choice of model-type and data used;
- This sensitivity is usually not specifically addressed (often calibrated away) and not properly and systematically documented in the many available published studies;
- The outcomes of such modelling exercises cannot be properly used when the underlying decisions on model and data type and sensitivities are unknown;
- Without this crucial knowledge regional crop simulation models can be easily miss-used by non-specialist;
- A standard decision procedure is proposed where these choices are documented in a standard format allowing cross comparisons of different approaches despite the often strong context dependency of the results.

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Annex

Description of modules in the LINTUL2-(FAST) and SUBSTOR-(DSSAT) that have been used in this thesis

SUBSTOR-potato model in DSSAT

In this thesis we used the SUBSTOR-potato model (Ritchie et al., 1995) to simulate variability in the productivity of potatoes as a function of environmental factors. The SUBSTOR-potato model (Ritchie et al., 1995) is available within the Decision Support System for Agro-technology Transfer (DSSAT) (Jones et al., 1998) and was calibrated and tested under Andean conditions as described by Stoorvogel et al. (2004) and Bowen et al. (1999). The SUBSTOR-potato model is one of 16 models embedded within the DSSAT (v4) program. A brief review of the SUBSTOR-Potato model is provided here for convenience but readers interested in a comprehensive description are referred to Griffin et al. (1993).

The SUBSTOR-Potato model simulates on a daily basis the growth and development of the potato crop using information on climate, soil, management and cultivar. The model is divided into four main sub models simulating simultaneously the phenological development, the biomass formation and partitioning, soil water and nitrogen balances to provide a realistic description of the plant–soil–atmosphere system. The phenological development is controlled by cumulative temperature whilst the growth rate is calculated as the product of absorbed radiation, which is a function of leaf area, using a constant ratio of dry matter yield per unit radiation absorbed. Cultivar-specific coefficients, also referred to as 'genetic coefficients', are used by the model to control tuber initiation, leaf area development, and tuber growth rate.

The soil water balance in DSSAT is based on Ritchie's model (Ritchie, 1981a, b) where the concept of drained upper limit and drained lower limit of the soil is used as the basis of the available soil water. This one dimensional and multi-layer model uses the 'tipping bucket' approach to compute the soil water drainage when a layer's water content is above a drained upper limit parameter (field capacity). The SCS method (Soil Conservations Service, 1972) modified to account for layered soil (Williams, 1984) is used to partition rainfall and/or irrigation into runoff and infiltration, based on a curve number that attempts to account for texture, slope, and tillage.

The nitrogen balance in the soil is simulated using the CERES N model where processes such as mineralization, immobilization, nitrification, de-nitrification, nitrogen uptake by plants, distribution and remobilization within the plants are simulated (Godwin and Singh, 1998). At each growth stage, deficits in soil water or nitrogen will affect the growth of the modelled crop and hence final yield. The model is designed to be used for simulation of two production levels. The potential yield production level is limited only by temperature, solar radiation and the specific physiological plant characteristics. At the water and nutrients-limited production level, the soil and plant water balance together with available nutrients are included in the simulation of potato growth.

LINTUL2 in FAST

LINTUL2 is a mechanistic crop growth simulation model that allows for the simulation of soft winter wheat under potential and water-limited conditions (for a comprehensive description: van Ittersum et al., 2003; Farré et al., 2000; Spitters and Schapendonk, 1990). LINTUL2 describes production under water-limited conditions by including a water balance of crop and soil in the LINTUL1 model. Conditions are still optimal with respect to other growth factors, i.e. ample nutrients and a pest-, disease- and weed-free environment. With the LINTUL2 model, options for water conservation can be studied, as well as differences among cultivars in drought tolerance.

The simple soil water balances in LINTUL2 are derived from more complex versions documented by Penning de Vries et al. (1989) and Stroosnijder (1982). Input data for the model are standard data of daily solar radiation, temperature and rainfall; plant density, dates of crop emergence and harvest; rootable depth; and the soil moisture retention characteristics, i.e. the relation between volumetric soil moisture content and suction. LINTUL2 has been used in numerous climate change studies (e.g. Hijmans, 2003; Wolf and van Oijen, 2002; Ewert et al., 1999; van Oijen and Ewert, 1999).

The model is integrated in Analysing Cropping systems and Environment (ACE) which is a further development of the recently developed cropping system modelling framework Agricultural Production and Externalities Simulator (APES) (Donatelli et al., 2010; van Ittersum et al., 2008).

The model was extended with a calibration algorithm and implemented to allow fast simulations (FAST; Fast Agro-Simulation Technique) for large numbers of spatial units and years with more than 100,000 runs per scenario for which temporal model performance becomes a critical issue. The resulting model LINTUL2 in FAST was further extended with various calibration methods under European conditions by Angulo et al. (2012) to allow the simulation of spatial and temporal yield trends and responses to climate change. A simple representation of the effects of increased atmospheric CO_2 level on biomass production was considered using the relationship between CO_2 level and radiation use efficiency as proposed by Stockle et al., (1992).

Moreover, a simple representation of the effects of technology development on biomass production using the estimation of yield changes due to improved varieties and crop management as described in (Ewert et al., 2005). Their results showed that the extended method considering the region-specific calibration of phenology and growth parameters is most suitable to simulate climate change effects on wheat yields in Western Germany (Angulo et al., 2012). The calibrated model LINTUL2 in FAST includes the effects of CO_2 levels and technology development on wheat production has been used in this thesis.

Table 1: Summary description of modules in the LINTUL2-(FAST) and SUBSTOR-(DSSAT)

Modules	Sub modules	Crop growth simulation model	
		LINTUL2-(FAST)	SUBSTOR-(DSSAT)
Weather		Reads or generates daily and/or hourly weather data: daily rainfall, maximum air, temperature, minimum air temperature, global solar radiation, wind speed, vapour pressure and Evapotranspiration	Reads or generates daily and/or hourly weather data: maximum and minimum temperatures, global radiation and precipitation
Soil	Soil moisture	Tipping bucket: drainage of water, runoff and irrigation are calculated in a preferential sequence in the tipping bucket model. Water uptake: Uptake of water from the soil by plant roots is driven by crop transpiration and may be modified by the amount of water in the profile.	Tipping bucket: snow accumulation and melt, runoff, infiltration, saturated flow and water table depth. Volumetric soil water content is updated daily for all soil layers.
	Soil carbon and nitrogen		Organic and inorganic fertilizer and residue placement decomposition rates, nutrient fluxes between various pools and soil layers. Soil nitrate and ammonium concentrations are updated on a daily basis for each layer.
	Soil temperature		Computes soil temperature by layer
	Soil dynamics		Computes soil structure characteristics by layer. This module currently reads values from a file, but future versions can modify soil properties in response to tillage.
Crop	Phenological development	Total crop growth: emergence and root growth take place only if there is enough water in the soil, i.e. if the water content is above wilting point. Crop growth rate is affected if the transpiration of the crop is hampered due to low water content in the rooted soil.	Define temperature effect on vegetative, early reproductive, and late reproductive development Parameters for each growth stage: preceding stage, photoperiod function, temperature function, temperature and water sensitivity, N and P sensitivity

	Formation of leaf, stem and root biomass and its partitioning,	Root-shoot partitioning: allocation of biomass over roots and shoot of the crop is changed if water stress occurs. The process is modelled in a general way, based on two assumptions: upon drought, more roots will be formed to alleviate the water shortage and thus less biomass is left for the shoot, the distribution of dry matter among stem, leaves and storage organs remains unchanged.	Dry matter partitioning to leaf, stem, and root as function of vegetative stage. Coefficients for partitioning at emergence, final growth stage, stem senescence, during water stress, and nodule growth Parameters that define leaf expansion response to temperature and solar radiation Initial root depth and length, root water uptake parameters Relative effects of temperature on pod set, seed growth and relative Change in partitioning Relative effects of soil water content.
Management operations module		Sowing and harvest dates. Technology development: yield changes due to improved varieties and crop management	Planting, emergence and harvest dates as well as about used amount of nitrogen, potassium and phosphorus fertilizers, irrigation and tillage practices and previous crop.

Summary

Modelling regional land use: the quest for the appropriate method

The demand for spatially-explicit predictions of regional crop-yield patterns is increasing. Policymakers need these predictions for e.g. regional development plans, the assessment of climate change impacts, and to reduce the threat of regional imbalances between food supply and demand (Lobell and Ortiz-Monasterio, 2007; De Wit et al., 2005; Jagtap and Jones, 2002). Agricultural census, other forms of direct surveys, or remote sensing imagery allow to assess spatial patterns of crop yield, but this will only provide insight ex post (Khan et al., 2010; Launay and Guerif, 2005). An alternative approach to assess a priori and/or future ranges of alternative scenarios spatial yield patterns at the regional scale is the application of mechanistic crop growth simulation models (e.g. Launary, 2002; Gomez and Ledoux, 2001; Faivre et al., 2000). However, two main problems emerge in the application of field-level CGSMs at regional scales. Firstly, the required input data on weather, soils, and management are often not available (data availability); and secondly, if they are, generally not at the required level of detail (data aggregation). As argued in Chapter 1, there are two possible approaches to address the identified problems. One is replacing the CGSM by a metamodel that is a simple mathematical function intended to mimic the behaviour of interest of a mechanistic model (Kleijnen and Sargent, 2000; Barton, 1998). The second approach is a simple empirical model that describe the response from observed crop yields (from e.g. survey data) to a range of explanatory (environmental and management) variables (e.g. Lobell et al., 2008).

The modelling-approach choices and performances are context dependent. The context conditions that determine the best approach are input data requirements, problem definition, study sub-objective, the scale at which output results are expected, model end-users, and utilization of the output (e.g. testing different scenarios). Since there will always be a certain level of idiosyncrasy to the case, one has to strive for a toolbox of approaches from which the proper tool can be selected on the basis of a number of specific criteria such as credibility, sensitivity, relevance, and user-friendliness. The selection of the modelling approaches can be considered as one of the most difficult, and often ignored, steps to model crop yield at the regional level. However, a structured, systematic way of modelling-approach selection is lacking. In order to address this issue this thesis aimed to develop a framework for recommendable practices to model regional patterns of crop yield. From this general objective, more specific sub-objectives are derived:

- To provide decision rules for selecting appropriate approaches to generate input variables to feed crop growth simulation models at the regional level;
- To provide decision rules for selecting appropriate procedure s to simulate regional yield patterns using crop growth simulation models (CGSMs);
- To identify, given context conditions, the most suitable modelling approach to simulate regional patterns of crop yield.

Chapter 2 discusses the issue of input data availability, reviews literature for existing approaches that have been used to overcome the problem of data availability. Then it uses the review to formulate decision rules as to what approach to take under different circumstances. Which of the approaches should be used depends on the following questions: (i) do observations of the input variable allow to estimate semivariograms?; (ii) are there auxiliary data correlated to the target variable?; (iii) do the input variables exhibit spatial correlation?; and (iv) is there spatial correlation in the residuals of the regression that related auxiliary data to the target variable?. Summarized, the selection of possible approaches depends on the data availability, the spatial variability, the temporal variability, the correlations with other variables, the data acquisition methods, the expected accuracy from a particular approach used to describe spatial variability, and the sensitivity of the CGSM to the variable. At the regional level CGSMs are typically fed by the input data that are generated as discrete zones. However, increasingly the input data are presented as continuous surfaces. This has the following reasons: (i) the surge of available auxiliary data including satellite images and DEMs; (ii) the accumulation of data sources (in digital form); and (iii) the development of interpolation techniques such as DSM that effectively uses auxiliary data. Generally, spatially-explicit regional patterns of yield are less accurate when done for discrete zones compared to continuous surfaces, although one should be aware of a false sense of accuracy, when continuous maps are made by unreliable interpolations. The most suitable method should be selected in a structural way, using decision rules as presented in Chapter 2.

Chapter 3 evaluates different procedures to simulate regional patterns of potato yields in the Carchi province in Northern Ecuador with field-level crop growth simulation models. It also examines scaling effects that arise from spatial variability in soil properties by using different supports. Results demonstrate that the order of calculation and interpolation was of major importance, while aggregation had a minor effect on the regional patterns of potato yield. The former is probability due to the non-linearity of the CGSM and the difference in the spatial dependency of individual inputs. The latter is probably due to the absence of local extremes, which is due to the gradual trends in soil properties in the volcanic ash soils of Carchi (being a result of the soil forming processes, but also a consequence of interpolation). The spatial comparison of regional patterns of crop yield shows that regional yield patterns generated by different procedures (i.e. different approaches and different supports) were similar, while, non-spatial comparisons of different yield patters in terms of the Root Mean Squared Differences showed better performance when calculations were performed first instead of staring with the interpolation of the input variables. From an uncertainty propagation and variability point of view it is in general preferable to calculate first before interpolation.

Chapters 4 and 5 compare and evaluate the performance of three different modelling approaches for their capacity to model regional patterns of crop yield for two different cases: potato yields in the Carchi province in Northern Ecuador (Chapter 4) and wheat yields in Western Germany (Chapter 5). Based on these findings, various criteria for selecting a modelling approach are defined including credibility, relevance, sensitivity, and user friendliness. The empirical model and the metamodel are very easy to use and transparent. However, their application domain is limited to the case study area. The application of the crop growth simulation model remains complex and the model functions as a black box. The strength of the CGSMs is that impacts over a wider range of conditions can be simulated, taking into account many factors in a way that would not be possible using empirical models and metamodels (Lobell and Burke, 2010; Bouman et al., 1998). It can be concluded that the various modelling approaches each have their unique merit. Hence, the different modelling approaches are therefore complementary for the interpretation of the observed patterns. There is not a single optimal solution to modelling agricultural systems to model, e.g. regional yield patterns. Moreover, Chapter 4 analyses the effect of spatial aggregation on the performance of the modelling approaches. The results showed that aggregation of calculated data leads to less variability and increasing linear fits at higher aggregation levels. The spatial variability in the case study area determines how strong this effect is.

Chapter 6 synthesises the methodologies and results from the research presented in this thesis. The chapter is divided into three main parts. The first part reflects upon the achievement of the specific research objectives. The second part synthesises the results of the thesis, and provides a framework for recommendable practices to model regional patterns of crop yield. The final conclusions are presented in the third part of the synthesis:

- Regional crop yield modelling is very sensitive to the choice of model-type and data used;
- This sensitivity is usually not specifically addressed and not properly and systematically documented in many studies;
- The outcomes of such modelling exercises cannot be properly used when the underlying decisions on model and data type and sensitivities are unknown;
- Without this crucial knowledge regional crop simulation models can be easily misused by non-specialists;
- Standard decision rules are proposed to document these choices in a standard format allowing cross comparisons of different approaches despite the often strong context dependency of the results.

Samenvatting

Het modelleren van regionale landgebruik: de zoektocht naar de juiste methode

De vraag naar ruimtelijk-expliciete voorspellingen van regionale patronen van gewasopbrengsten neemt toe. De politiek heeft deze voorspellingen nodig voor o.a. regionale ontwikkelingsplannen, het inschatten van de gevolgen van klimaatsverandering, en om de bedreiging van een regionale onbalans tussen het aanbod en de vraag naar voedsel te verminderen (Lobell en Ortiz-Monasterio, 2007; De Wit et al., 2005; Jagtap en Jones, 2002). De landbouwcensus, maar ook andere vormen van enquêtes of aardobservatie, maken het mogelijk om ruimtelijke patronen van gewasopbrengsten te analyseren. Dit geeft echter alleen inzichten ex post (Khan et al., 2010; Launay en Guerif, 2005). Een alternatieve methode om a priori onder alternatieve scenario's de ruimtelijke patronen op regionale schaal in te schatten is met behulp van mechanistische gewasgroeimodellen (e.g. Launary, 2002; Gomez en Ledoux, 2001; Faivre et al., 2000). Omdat de gewasgroeimodellen op veldniveau zijn ontwikkeld, leidt hun inzet op regionale schaal tot twee problemen. Ten eerste, zijn de benodigde invoergegevens m.b.t. weer, bodem, en management vaak niet beschikbaar. Ten tweede, hebben de invoergegevens, als ze al beschikbaar zijn, vaak niet het gewenste schaalniveau. Zoals aangegeven in hoofdstuk 1, zijn er twee mogelijke manieren om de verschillende problemen aan te pakken. Eén optie is om het gewasgroeimodel te vervangen door een metamodel. Een metamodel is een simpele mathematische functie die het gedrag van een mechanistisch gewasgroeimodel imiteert (Kleijnen en Sargent, 2000; Barton, 1998). Een alternatieve aanpak is om een simpel empirisch model te ontwikkelen dat waargenomen gewasopbrengsten (van bijv. enquêtes) aan verklarende factoren koppelt (e.g. Lobell et al., 2008).

De keuze van modelaanpak en hun prestatie zijn context specifiek. De omstandigheden die bepalen welk model de beste resultaten geeft worden bepaald door de beschikbare invoergegevens, de onderzoeksvraag, het gewenste schaalniveau, en het gebruik van de eindresultaten (bijv. het testen van scenario's). Aangezien case-studies altijd specifiek zijn en moeilijk te generaliseren, moet men streven naar een set van verschillende aanpakken van waaruit op basis van verschillende criteria zoals geloofwaardigheid, gevoeligheid, relevantie, en gebruikersvriendelijkheid geselecteerd kan worden. De selectie van modelaanpak kan gezien worden als één van de moeilijkste, en vaak genegeerde, stappen om gewasopbrengsten op het regionaal niveau te modelleren. Een gestructureerde manier om deze keuze te maken mist echter nog. Om hier beter mee om te gaan, richt dit proefschrift zich op een raamwerk waarmee de beste aanpak om regionale patronen van gewasopbrengsten te modelleren geselecteerd kan worden. Van deze algemene doelstelling zijn een aantal specifieke doelstellingen afgeleid:

- Het ontwikkelen van beslissingsregels om geschikte methodes te selecteren voor het genereren van invoervariabelen om de simulatiemodellen voor gewasgroei op regionaal niveau te voeden;
- Het ontwikkelen van beslissingsregels voor de selectie van de juiste procedures om patronen van gewasopbrengsten te simuleren met modellen voor gewasgroei;
- Het opzetten van procedures om, gegeven een bepaalde context, het meest geschikte modeltype te selecteren om regionale patronen van gewasopbrengst te simuleren.

Hoofdstuk 2 bediscussieerd de kwestie van de beschikbaarheid van invoergegevens en analyseert de literatuur voor methodes die gebruikt zijn om problemen met gegevensbeschikbaarheid op te lossen. Dit overzicht is vervolgens het startpunt om beslissingsregels te formuleren die helpen de juiste methode te selecteren voor bepaalde omstandigheden. Deze keuze hangt af van de volgende vragen: (i) laten waarnemingen van de inputvariabele het toe om een semi-variogram te schatten?; (ii) zijn er hulpvariabelen beschikbaar die gecorreleerd zijn aan de doelvariabele?; (iii) zijn de invoergegevens ruimtelijk gecorreleerd?; en (iv) zijn de residuen van de regressie tussen doelvariabele en hulpvariabele ruimtelijk gecorreleerd? Samenvattend hangt de selectie van mogelijke methodes af van de databeschikbaarheid, de ruimtelijke variabiliteit, de temporele variabiliteit, de correlaties met andere variabele, de gevraagde nauwkeurigheid om de ruimtelijke variabiliteit te beschrijven en de gevoeligheid van het gewasgroeimodel voor de variabele. Op het regionaal niveau worden de invoergegevens voor gewasgroeimodellen vaak beschreven door middel van discrete zones. In toenemende mate worden de gegevens echter steeds vaker beschreven als continue oppervlaktes. Hiervoor zijn een aantal redenen aan te wijzen: (i) de snelle groei aan beschikbare secundaire data zoals satellietbeelden en digitale hoogtemodellen; (ii) de toename aan verschillende bronnen met (digitale) gegevens; en (iii) de ontwikkeling van interpolatietechnieken zoals digitale bodemkarteringen die effectief gebruik maken van secundaire data. In het algemeen zijn regionale patronen van gewasopbrengsten minder nauwkeurig als ze afgeleid zijn discrete zones in vergelijking tot continue oppervlaktes. Het zou echter een vals gevoel van nauwkeurigheid kunnen zijn omdat continue oppervlaktes gemaakt kunnen zijn door onnauwkeurige interpolaties. Het is daarom van belang om de beste methodes te selecteren in een gestructureerd manier, zoals door het gebruik van de beslissingsregels gepresenteerd in hoofdstuk 2.

Hoofdstuk 3 evalueert verschillende procedures voor het simuleren van regionale patronen van aardappel opbrengst in de provincie Carchi in Noord-Ecuador met simulatie modellen voor gewasgroei ontwikkeld op veldniveau. Er wordt ook ingegaan op de schaal effecten die voortvloeien uit de ruimtelijke variabiliteit van de gebruikte bodem eigenschappen. Resultaten tonen aan dat de volgorde van de berekening en de interpolatie van groot belang was. Aggregatie van invoer of uitvoergegevens had een gering effect op de regionale patronen van de aardappel opbrengst. De verschillen in de volgorde van de methodes zijn waarschijnlijk te wijten aan de niet-lineariteit van het simulatiemodel en het verschil in ruimtelijke afhankelijkheid van de afzonderlijke invoergegevens. Aggregatie heeft weinig effect vanwege de afwezigheid van lokale extremen, die door de geleidelijke ontwikkeling van bodemeigenschappen in de vulkanische as bodems van Carchi (welke een gevolg zijn van de bodem vormingsprocessen, maar ook een gevolg van de gebruikte interpolatietechniek). Uit de ruimtelijke vergelijking van regionale patronen van gewasopbrengst blijkt dat de regionale opbrengst patronen gegenereerd door verschillende procedures (d.w.z. verschillende benaderingen en verschillende gegevens) vergelijkbaar waren, terwijl, niet-ruimtelijke vergelijkingen van verschillende opbrengst patronen in termen van bijv. de *Root Mean Squared Difference* betere prestaties vertonen van de aanpak waarbij eerst gesimuleerd wordt in vergelijking met de procedure waar eerst geïnterpoleerd wordt. Vanuit het oogpunt van foutenvoortplanting en variabiliteit is het in het algemeen beter om eerst te simuleren voor punten waarna de resultaten geïnterpoleerd worden.

De hoofdstukken 4 en 5 vergelijken en evalueren de prestaties van drie verschillende modellen op basis van hun capaciteit om regionale patronen van gewasopbrengst te modelleren in twee verschillende studies: aardappel opbrengsten in de Carchi provincie in het noorden van Ecuador (hoofdstuk 4) en tarwe opbrengsten in West-Duitsland (Hoofdstuk 5). Op basis van de resultaten zijn criteria gedefinieerd voor het selecteren van de beste modelaanpak, waaronder geloofwaardigheid, relevantie, gevoeligheid, en gebruiksvriendelijkheid. Empirische modellen en metamodellen zijn zeer makkelijk te gebruiken en transparant. Echter, hun toepassingsdomein is beperkt tot het studiegebied.

De toepassing van simulatiemodellen voor gewasgroei blijft complex en de modellen functioneren vaak als een zwarte doos. Echter, de kracht van de simulatiemodellen is dat effecten over een breder scala van omstandigheden gesimuleerd worden. Daarnaast houden ze rekening met veel factoren op een wijze die niet mogelijk zou zijn met empirische modellen en metamodellen (Lobell en Burke, 2010; Bouman et al., 1998). Geconcludeerd kan worden dat de verschillende modellen elk hun eigen verdienste hebben. Vandaar dat de verschillende modelmatige benaderingen elkaar mooi aanvullen om waargenomen patronen te interpreteren. Door de grote verschillen tussen case studies, is er geen optimale methode om landbouwsystemen te modelleren. Hoofdstuk 4 laat ook nog het effect van ruimtelijke aggregatie op de prestaties van de modelleringsbenaderingen zien. De resultaten tonen aan dat de aggregatie van de berekende gegevens de variabiliteit vermindert en lineaire relaties met verklarende factoren op hogere aggregatieniveaus verbeteren. De ruimtelijke variabiliteit in het studiegebied bepaalt hoe sterk dit effect is.

Hoofdstuk 6 synthetiseert de methoden en de resultaten van het onderzoek beschreven in dit proefschrift. Het hoofdstuk bestaat uit drie delen. Het eerste deel reflecteert op de verwezenlijking van de specifieke doelstellingen van het onderzoek. Het tweede deel synthetiseert de resultaten van het proefschrift, en biedt een kader voor de aan te bevelen praktijken om regionale patronen van de gewasopbrengst. De definitieve conclusies worden gepresenteerd in het derde deel van de synthese:

- Het modelleren van regionale gewasopbrengsten is zeer gevoelig voor de keuze van het model-type en de gebruikte gegevens;
- In tal van studies is deze gevoeligheid meestal niet specifiek behandeld en niet goed en systematisch gedocumenteerd;
- De uitkomsten van de modelstudies kunnen niet goed worden gebruikt wanneer de onderliggende keuzes m.b.t. model en data type en de gevoeligheden onbekend zijn;
- Zonder deze essentiële kennis kunnen regionale simulatiemodellen voor gewasgroei eenvoudig worden misbruikt door niet-specialisten;
- Standaard beslisregels worden voorgesteld om deze keuzes te documenteren in een standaardformaat. Hierdoor kunnen verschillende benaderingen vergeleken worden, ondanks de vaak sterke context-afhankelijkheid van de resultaten.

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About the author

Curriculum Vitae

Afsaneh Soltani Largani, 30 November 1972, Tehran, Iran.

BSc in Environmental Science, Faculty of Natural Resources, 22 September 1997, Tehran University, Iran.

MSc in Environmental Science, Faculty of Natural Resources, 12 February 2000, Tehran University, Iran.

PhD in Environmental Science, Soil Geography and Landscape Group, 28 August 2013, Wageningen University, The Netherlands.

E-mail: asllsoltani@yahoo.com

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Conference contributions

Soltani, A. and Stoorvogel, J.J. 2011. The application of crop growth simulation models and pesticide leaching models on a regional scale. The Annual North American Agroforestry conference, June 4-9, Athens, Georgia, USA.

Soltani, A., Bakker, M.M. and Stoorvogel, J.J. 2011. Using temporal and spatial analogues to simulate climate change effects on European crop production. 1th International conference on Food and Environment, June 21-23, The New Forest, UK.

PE&RC PhD Education Certificate

With the educational activities listed below the PhD candidate has complied with the educational requirements set by the C.T. de Wit Graduate School for Production Ecology and Resource Conservation (PE&RC) which comprises of a minimum total of 32 ECTS (= 22 weeks of activities)

Review of literature (4.5 ECTS)

- Review on assessing regional production (2007)

Writing of project proposal (4.5 ECTS)

- Reduced-complexity modelling for integrated assessment of land use systems (2007)

Post-graduate courses (9 ECTS)

- Land science course; PE&RC, Kenya (2009)
- Environmental research in context (A1); WIMEK (2006)
- Monitoring of natural hazards from space; Alpabach, Austria (2006)
- Wisconsin entrepreneurial bootcamp; Madison, USA (2010)

Deficiency, refresh, brush-up courses (15 ECTS)

- Environment and society (2006)
- Environmental systems analysis: methods and Application (2006)
- Remote sensing (2007)

Competence strengthening / skills courses (3.3 ECTS)

- EndNote 8; WGS (2006)
- Techniques for writing and presenting a scientific paper; WGS (2009)
- Project and time management; WGS (2010)

- The art of modelling (2007)
- Uncertainty propagation in spatial and environmental modelling (2007)
- Physical modelling (2007)
- Basic statistics (2007)
- C++ for Biologists (RSEE) (2006)

PE&RC Annual meetings, seminars and the PE&RC weekend (1.2 ECTS)

- PE&RC Weekend (2009)
- PE&RC Day (2009)

Discussion groups / local seminars and other meetings (6 ECTS)

- Natural resources seminar: environmental assessment of Chalous river's damn, tunnel & channel by geographic information system (2008)
- Natural resources seminar: categorizing various parks in accordance with determinative species by fax-pro (2008)
- Spatial methods (SPAM) (2009, 2010)

International symposia, workshops and conferences (4.7 ECTS)

- The Annual North American Agroforestry conference, Athens, Georgia, USA (2011)
- First International Conference on Food and Environment, The New Forest, UK (2011)

Lecturing / supervision of practical's / tutorials (4.5 ECTS)

- Land degradation and economic development; 3 weeks (2008)

PE&RC Annual meetings, seminars and the PE&RC weekend (1.2 ECTS)

- PE&RC Weekend (2009)
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