Root-restricting layers in German agricultural soils

Extent, cause and management strategies

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Abstract

Subsoil, i.e., soil below 30 cm depth, harbours great amounts of water and nutrients. However, physical and chemical barriers for vertical root elongation may restrict plants from accessing subsoil resources. Such root-restricting soil layers (**RRLs**) were subject of the present thesis. Focusing on agricultural soils in Germany, the major aims of this thesis were to (i) identify the main soil-borne **causes** for restricted vertical root elongation, (ii) examine the **effects** of RRLs on the productivity function and carbon (C) storage function of soil, (iii) quantify the contribution of anthropogenically compacted soil to the spatial **extent** of RRLs, and (iv) evaluate **management** strategies for agricultural soil with RRLs.

Most of this thesis has evolved from data of the first German Agricultural Soil Inventory (2011–2018), which comprises information on the soil and management at 3104 sites covering all agricultural land in Germany in a regular 8 km x 8 km grid. For describing the cause and extent of root restriction, literature was reviewed for threshold values, which were subsequently validated with root count data from the inventory. Effects of RRLs on the productivity function and C storage function of soil were examined by comparing yield of winter wheat and depth gradients of organic C densities at different magnitudes of root restriction (inventory data). Additionally, a global meta-analysis of long-term field experiments was carried out to compare yield of annual crops growing on sites with RRLs to adjacent sites where RRLs were previously meliorated by deep tillage. Anthropogenic soil compaction in German agricultural soils was quantified with a novel, data-driven approach. Management options were examined in a literature review and the popularity of these options was assessed based on the inventory.

The dominant soil-borne cause for restricted elongation of deep roots was high compactness – almost half (46 %) of German agricultural land was compacted to an extent that restricted root growth. Other causes included groundwater-induced anoxia (14 % of agricultural land), sandy subsoil texture (12 %), acidity (10 %), large rock fragment content (8 %), shallow bedrock (6 %), and cementation (2 %). These RRLs significantly decreased the productivity function of soils. In the meta-analysis of long-term field experiments, RRLs decreased yield of annual crops on average by about 20 %. On German farms, grain yield of winter wheat was on average 0.5 Mg ha^{-1} (6 %) lower in the presence of severe RRLs compared to reference sites without RRLs. Most RRLs were of pedogenic ("natural") origin with RRLs being significantly more prevalent in Podzols, Gleysols and Vertisols than in other soil groups. However, anthropogenic compaction has significantly increased

the spatial extent of RRLs in German agricultural soils. About 10 % of cropland was estimated to be compacted due to traffic, 1 % due to organic C loss-induced collapse of soil structure, and further 2 % due to a combination of both factors. German farmers either accepted the presence of RRLs and adapted land use and management accordingly or they meliorated affected sites. Melioration measures included drainage (45 % of agricultural land), deep loosening (6 % at least once within ten years prior to sampling), deep ploughing (5 % at least once in history), and liming to correct soil acidity (54 %).
In the upper metre of German agricultural soils, about 30 % of the available water capacity, 30 % of total phosphorus and 20 % of total nitrogen resources were hidden below RRLs. Thus, the melioration of RRLs could significantly improve plant nutrition. Furthermore, the melioration of RRLs could increase the transfer of atmospheric C into the subsoil via deep roots and increase soil C storage. It was estimated that compacted cropland with packing densities $> 1.75\,\mathrm{g\,cm^{-3}}$ could store up to $2.3\,\mathrm{Mg\,ha^{-1}}$ more organic C in 30–100 cm if sustainably meliorated (loosened). However, not every soil is capable of being meliorated. In terms of a sustainable bioeconomy, it is therefore of central importance to stop the further spread of RRLs and prevent traffic-induced soil compaction.

Zusammenfassung

Ein großer Anteil der im Boden gespeicherten Nährstoff- und Wasser-Ressourcen befindet sich im Unterboden, d. h. im Bodenmaterial unterhalb 30 cm Tiefe. Jedoch sind diese oft nur begrenzt pflanzenverfügbar, da Wurzeln aufgrund eingeschränkter Gründigkeit nicht bis in den Unterboden einzudringen vermögen. Die vorliegende Arbeit handelt von der Durchwurzelbarkeit landwirtschaftlich genutzter Böden. Mit Blick auf Deutschland sollte untersucht werden, (i) welche Bodeneigenschaften die Durchwurzelbarkeit einschränken, (ii) wie sich die eingeschränkte Durchwurzelbarkeit auf Produktivitäts- und Kohlenstoffspeicherfunktionen von Böden auswirkt, (iii) wie sehr anthropogene Schadverdichtung zur Verbreitung eingeschränkt durchwurzelbarer Böden beigetragen hat, und (iv) wie die Bewirtschaftung schlecht durchwurzelbarer Böden optimiert werden kann.

Der größte Teil der vorliegenden Arbeit beruht auf Auswertungen der Bodenzustandserhebung Landwirtschaft (BZE-LW), im Rahmen derer zwischen 2011 und 2018 Boden- und Bewirtschaftungsdaten von insgesamt 3104 Acker-, Grünland-, und Dauerkultur-Standorten in einem 8 km x 8 km Raster erhoben wurden. Zur Bewertung der Durchwurzelbarkeit wurden internationaler Fachliteratur Schwellenwerte entnommen, welche anhand von Wurzel-Erhebungen der BZE-LW überprüft wurden. Um Effekte von Durchwurzelbarkeit auf die Produktivitäts- und Kohlenstoffspeicherfunktionen von Böden abzuschätzen, wurden Kornerträge von Winterweizen sowie Kohlenstoffvorräte von Standorten mit unterschiedlich stark eingeschränkter Durchwurzelbarkeit miteinander verglichen (BZE-LW). Zusätzlich wurde eine globale Meta-Analyse von Dauerfeldversuchen mit Ertragsdaten von Flächen mit eingeschränkter Durchwurzelbarkeit und benachbarten Flächen mit verbesserter (meliorierter) Durchwurzelbarkeit durchgeführt. Managementoptionen für eingeschränkt durchwurzelbare Böden wurden anhand einer Literaturstudie eruiert und die Popularität dieser Optionen wurde auf Grundlage der BZE-LW bewertet.

Auf fast der Hälfte (46 %) der landwirtschaftlichen Nutzfläche Deutschlands schränkte ein besonders dicht gelagertes Bodengefüge die Durchwurzelbarkeit ein – weitere Ursachen waren grundwasserinduzierter Sauerstoffmangel (14 %), sandige Unterbodentextur (12 %), starke Versauerung (10 %), hoher Skelettanteil (8 %), anstehendes Festgestein (6 %) und verkittetes Bodengefüge (2 %). In der globalen Meta-Analyse von Dauerfeldversuchen

zeigten einjährige Ackerkulturen auf schlecht durchwurzelbare Böden durchschnittlich um etwa 20 % niedrigere Erträge als benachbarte, meliorierte Flächen. Auf deutschen Äckern waren die Kornerträge von Winterweizen bei stark eingeschränkter Durchwurzelbarkeit durchschnittlich um 0.5 Mg ha^{-1} (6 %) geringer als auf normal durchwurzelbaren Referenzböden. Einschränkungen der Durchwurzelbarkeit waren zumeist pedogenen ("natürlichen") Ursprungs. Jedoch haben auch anthropogene Schadverdichtungen signifikant zur Verbreitung schlecht durchwurzelbarer Ackerböden beigetragen. Es wird geschätzt, dass etwa 10 % der deutschen Ackerfläche durch Befahrung schadverdichtet wurde, 1 % durch den Verlust organischer Bodensubstanz, und weitere 2 % in Kombination beider Faktoren. In der landwirtschaftlichen Praxis wurde entweder das Vorhandensein eingeschränkter Durchwurzelbarkeit akzeptiert und Landnutzung sowie Bewirtschaftung daran angepasst, oder die betroffenen Standorte wurden melioriert. Zu den Meliorationsmaßnahmen gehörten Drainage (45 % der landwirtschaftlichen Nutzfläche), Tiefenlockerung (6 % mindestens ein Mal in 10 Jahren vor Probennahme), Tiefpflügen (5 % mindestens ein Mal) und Aufkalkung (54 %).
Etwa 30 % der nutzbaren Feldkapazität, sowie jeweils 30 % und 20 % der im oberen Meter gespeicherten Gesamtvorräte an Phosphor und Stickstoff verbargen sich unterhalb des durchwurzelbaren Bodenraumes. Meliorationsmaßnahmen zur Förderung der Durchwurzelbarkeit könnten die Pflanzenernährung stark verbessern. Darüber hinaus könnten Meliorationen den Eintrag wurzelbürtigen Kohlenstoffs in den Unterboden und somit dessen Kohlenstoffspeicherfunktion stärken. Es wird geschätzt, dass durch Gefügemelioration von Ackerböden mit effektiven Lagerungsdichten > 1.75 g cm^{-3} bis zu 2.3 Mg ha^{-1} zusätzlich in 30–100 cm gespeichert werden könnten. Jedoch ist nicht jeder Boden meliorationsfähig. Im Sinne einer nachhaltigen Bioökonomie ist es deshalb von zentraler Bedeutung, eine weitere Ausbreitung schlecht durchwurzelbarer Böden zu verhindern und Bodenschadverdichtung durch gute fachliche Praxis zu vermeiden.

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List of Abbreviations

AUC	Area under the curve
CART	Classification and regression tree
CI	Confidence interval
MOC	Mineral-associated organic carbon
MSE	Mean square error
OLS	Ordinary least squares regression
PD	Packing density
POC	Particulate organic carbon
PTF	Pedo-transfer function
QR	Linear quantile regression
$\mathbf{R}^2$	Coefficient of determination
RMSE	Root mean square error
ROC	Receiver operating characteristic
RRL	Root-restricting soil layer
RSS	Residual sum of squares
RY	Relative yield
TIC	Total inorganic carbon
TOC	Total organic carbon
WRB	World Reference Base

Chapter 1

General introduction

1.1 Rationale

During the past decades, the German agricultural sector has undergone a remarkable change. In 1960, each German farmer produced enough food to feed about 17 people (BLE, 2019). Today, 60 years later, this number has risen to 140 (BLE, 2019). In the same time period[1], yield of the staple crop wheat has increased 2.4-fold, so did milk yield (FAO, 2020). Today, each hectare wheat produces on average 7.7 $\mathrm{Mg\,year^{-1}}$ of grain and each cow gives 7.8 $\mathrm{Mg\,year^{-1}}$ of milk (FAO, 2020). This increase in productivity was driven by technological advances, specialisation of farms and global trade. Germany currently ranks third in both global agricultural exports and imports (BMEL, 2019). Exports mainly comprise dairy products and pork, while about one quarter of the proteins contained in animal feed are imported (BMEL, 2019).

Agricultural intensification forms the backbone of today's food security and social prosperity. However, the increase in productivity has also been accompanied by costs to the environment, for which German farmers are increasingly criticised. Many agricultural soils in Germany are over-fertilised, especially in regions with concentrated dairy production and animal husbandry (UBA, 2019b). Global trade among highly specialised farms has fostered a regional imbalance in the distribution of soil nutrients. Farms specialising on livestock production tend to import many more nutrients within fodder than is being exported in the form of meat or dairy products, which is why their fields are often over-fertilised (UBA, 2019b). If nutrient applications to soil exceed plant uptake, a large proportion of the excess nutrients eventually end up in waterbodies, which causes eutrophication and high costs for purifying drinking water. Another point of criticism are greenhouse gas

[1] The following numbers represent mean values from 1961 to 1965 (past) and 2014 to 2018 (today)

emissions associated with animal husbandry, nitrogen fertilisation and peatland cultivation. During the past decade, these emissions have been rising – agriculture currently accounts for 11 % of German greenhouse gas emissions (UBA, 2019a). But the agricultural sector does not only contribute to climate change, it is also threatened by it. In recent decades, the frequency and intensity of droughts has been increasing causing significant yield losses (Lüttger & Feike, 2018). In the future, dry spells will likely be amplified further (Samaniego et al., 2018).
In order to make Germany's bioeconomy more sustainable, future agricultural food and fibre production needs to (i) cope better with drought stress, (ii) decrease greenhouse gas emissions, and (iii) reduce fertiliser applications without compromising yield. **Deeper rooting crops** could contribute to achieving all three of these goals (Lynch & Wojciechowski, 2015). Deep roots can access plant-available water resources from subsoils long after topsoils have dried out (Barraclough et al., 1989; Kirkegaard et al., 2007). They transfer atmospheric carbon (C) into the subsoil, which can increase soil organic C storage on the long term, and thus mitigate anthropogenic greenhouse gas emissions (Kell, 2011, 2012; Lynch & Wojciechowski, 2015). Finally, deep roots can decrease leaching losses of mobile nutrients like nitrate, increasing fertiliser use efficiency (Dunbabin et al., 2003; Lynch, 2013) and plants with deep roots can profit from involving subsoil repositories in nutrient cycling (Bauke et al., 2018; Kautz et al., 2013).

But how to achieve deeper rooting? On the one hand, root architecture is genetically controlled and deeper rooting can be achieved by crop selection and breeding (Lynch & Wojciechowski, 2015). However, root growth is also highly responsive to its environment (Kolb et al., 2017), which gives rise to a huge developmental plasticity of roots in soils (Wasson et al., 2014; Vetter & Scharafat, 1964). It is widely agreed that certain soil properties restrict root elongation of most cultivated plants. Such **root-restricting soil properties** are subject of the present thesis.

1.2 State of the art

1.2.1 What are root-restricting soil layers?

There is a wide scientific consensus about the presence of root-restricting soil properties. Depths to root-restricting layers (RRLs) are commonly recorded in soil surveys worldwide. In the soil survey manual of the United States Department of Agriculture, root-restricting depth is defined as the "depth at which physical [...] and/or chemical characteristics strongly inhibit root penetration", and restriction is characterised as "the incapability [of soil] to support more than a few fine or very fine roots if the depth from the soil surface and the water state [...] are not limiting" (Soil Science Division Staff, 2017). In German-speaking countries, the term "Gründigkeit" is commonly used to describe root-restricting soil depth: "Unter [...] Gründigkeit wird die Tiefe verstanden, bis zu der die Pflanzenwurzeln unter den gegebenen Verhältnissen tatsächlich in den Boden einzudringen vermögen" (AD-HOC-AG Boden, 2005).

RRLs are typically identified based on morphological traits of soil profiles. In the USA, bedrock as well as cemented and compacted soil layers, such as duripans and fragipans, are classified as barriers for root growth (Soil Science Division Staff, 2017). In Germany, groundwater-induced anoxia and sudden changes of chemical properties tend to be additionally considered as root-restricting (AD-HOC-AG Boden, 2005). In Switzerland, rock fragments are also accounted for when assessing the elongation potential of roots in soil (BGS, 2010). This illustrates that, although soil scientists worldwide acknowledge the presence of root-restricting soil properties, existing definitions of RRLs remain vague. Differences in defining RRLs do not only exist on the national level, but also between individual soil scientists. Soil survey manuals tend to give qualitative descriptions of RRLs that can be evaluated based on visual-tactual observations of soil profiles – this is easy because it does not require additional tools. But a quantitative characterisation of RRLs based on measured data would make their identification less biased and increase the comparability among sites.

Leenaars et al. (2018) reviewed indicators and associated threshold values for mapping rootable soil depths in sub-Saharan Africa. However, such a framework cannot simply be applied in target regions with different environmental conditions. Also, the type of data available to describe RRLs can vary substantially between regions of interest. For these reasons, there is a need to conduct further region-specific investigations. **A quantitative framework to characterise RRLs, which is optimised for agricultural soils in Germany, has not yet been developed**.

1.2.2 Why care about root-restricting soil layers?

In healthy soil without RRLs, the water and nutrient resources stored in subsoil provide an important insurance system to plants. During droughts, subsoil water can sustain plant growth long after topsoils have already dried out (e.g., Kirkegaard et al., 2007). And, to a certain degree, subsoil nutrients can sustain the productivity of agro-ecosystems even if nutrient resources in topsoil alone would be limiting growth (Kuhlmann & Baumgärtel, 1991). Deep roots allow mobile nutrients such as nitrate to be better captured, and thus extend the time period during which the applied nitrogen fertiliser is available to plants (Dunbabin et al., 2003; Lynch, 2013). Under heavy nitrogen fertilisation, deep roots take up significant amounts of leached nitrate from subsoils, along with phosphorus (Bauke et al., 2018). In restricting the ability of plants to tap water and nutrient reserves from the subsoil, RRLs limit the fertility, i.e., productivity function, of soils. I assume this to be the main reason for RRLs to be commonly recorded in soil surveys worldwide. However, to the best of my knowledge, there is **no study yet that has actually quantified the effects of RRLs on the productivity function of soils at a regional scale**.

The limited productivity function of soils is one reason for RRLs to be examined. Another reason is that RRLs could limit the function of soils to store organic C (Lynch & Wojciechowski, 2015). Soils are an important compartment of the global C cycle, storing about twice the amount of C that currently resides in the Earth's atmosphere as carbon dioxide (IPCC, 2013). The C pools of both compartments, pedosphere and atmosphere, are in a state of dynamic equilibrium. Shifting this equilibrium towards soil C could mitigate greenhouse gas-induced global warming (Minasny et al., 2017). Considering that (i) most soil organic C is assumed to be root-derived (Rasse et al., 2005), and (ii) RRLs restrict the rootability of subsoil, RRLs should also restrict the organic C stock of subsoil. However, the hypothesised **negative effect of RRLs on the organic C stock of subsoil still remains to be validated** under field conditions.

1.2.3 Has traffic-induced soil compaction increased the spatial extent of root-restricting layers?

The increase in agricultural productivity was fostered by large technological advances of agricultural machinery. For example, it was not until the 1960s, that combine harvesters were introduced on German farms at large scale. These early combine harvester processed about 4 Mg of wheat per hour (Schjønning et al., 2015), which was already much more than what had been achieved by manual labour before. The latest combine harvester model of the current market leader in western Europe, can even process more than 80 Mg of wheat per hour[2]. However, this 20-fold increase in productivity was also associated with significant increases of vehicle loads. Modern combine harvesters weigh more than 30 Mg when fully loaded[3]. Trafficking soil with such heavy machinery can cause severe soil compaction (Keller et al., 2019). This has been confirmed, for example, by Mordhorst et al. (2019) who observed the wide-spread occurrence of traffic-induced platy soil structures in northern Germany. Soil compaction restricts the potential of roots to elongate through soil. Therefore, traffic-induced compaction might have increased the spatial extent of RRLs in German agricultural soils in recent decades. However, **representative empirical data quantifying the extent and severity of anthropogenic compaction for all German agricultural soils does not yet exist.**

1.2.4 How to manage sites with root-restricting soil layers?

Farmers may accept the presence of RRLs and adapt cultivation practices accordingly. Or they can try to meliorate affected sites. Depending on the cause of restricted rooting, different melioration options are available. For example, mechanical loosening by deep tillage has been practiced in an attempt to meliorate compacted subsoil layers (Schulte-Karring, 1970a). However, **long-term field experiments examining the effect of meliorative deep tillage on crop yield delivered inconsistent findings** of which a comprehensive overview is still missing to date. Also, **little is known about the popularity of deep tillage and other management strategies for dealing with RRLs in practice**.

1.3 Research questions

In this thesis, I examine soil properties that impede the vertical elongation of deep roots and therefore restrict the plant-availability of water and nutrient ressources from subsoils. I discuss causes of such root-restricting soil layers (RRLs)

[2] `https://go.claas.com/lexionworldrecord` (last accessed 29th May 2020)
[3] `https://www.claas.de/produkte/maehdrescher/lexion-8900-7400` (last accessed 29th May 2020)

and management strategies for agricultural soils with barriers for root growth. Furthermore, I evaluate effects of RRLs on the functioning of agricultural soils in Germany. Specifically, the following research questions are addressed:

1) Which site properties impede root growth in German agricultural soils?

2) To what extent do RRLs limit the productivity function of agricultural soils?

3) Do RRLs limit the organic C storage function of agricultural soils?

4) Has anthropogenic soil compaction increased the spatial extent of RRLs in German agricultural soils?

5) How do farmers manage agricultural soils with RRLs in Germany?

6) How does meliorative deep tillage affect crop yield?

Most of this thesis is based on data from the first German Agricultural Soil Inventory (2011–2018), which comprises information on the soil and management at 3104 sites covering all cropland and grassland in Germany in a regular 8 km x 8 km grid (Jacobs et al., 2018; Poeplau et al., subm) (Fig. 1.1). In chapter 2, a quantitative framework is developed for characterising RRLs based on threshold values from the literature and this framework is validated with root count data from the inventory. Grain yield data recorded within the German Agricultural Soil Inventory provided the basis for examining the effect of RRLs on the productivity function of soils (chapter 2). Anthropogenic soil compaction in German agricultural soils was quantified with a novel, data-driven approach, which is also presented as part of chapter 2. For examining the effect of RRLs on the organic C storage function of soils, novel data on organic C quality (density fractions, $\delta^{13}C$ and $\delta^{15}N$) was aligned to data from the German Agricultural Soil Inventory (chapter 3). In chapter 4, adaptation and melioration strategies are discussed for cultivating soils with RRLs and, again, data from the German Agricultural Soil Inventory is used to examine the popularity of these management options. Finally, chapter 5 comprises a global meta-analysis of long-term field experiments about the effects of meliorative deep tillage on crop yield from sites with different magnitudes of root-restriction and climate.

For answering the research questions of the present thesis, machine learning with Random Forest algorithms played a key role. Before starting with the main chapters, I will now briefly introduce Random Forest algorithms and illustrate why they were used.

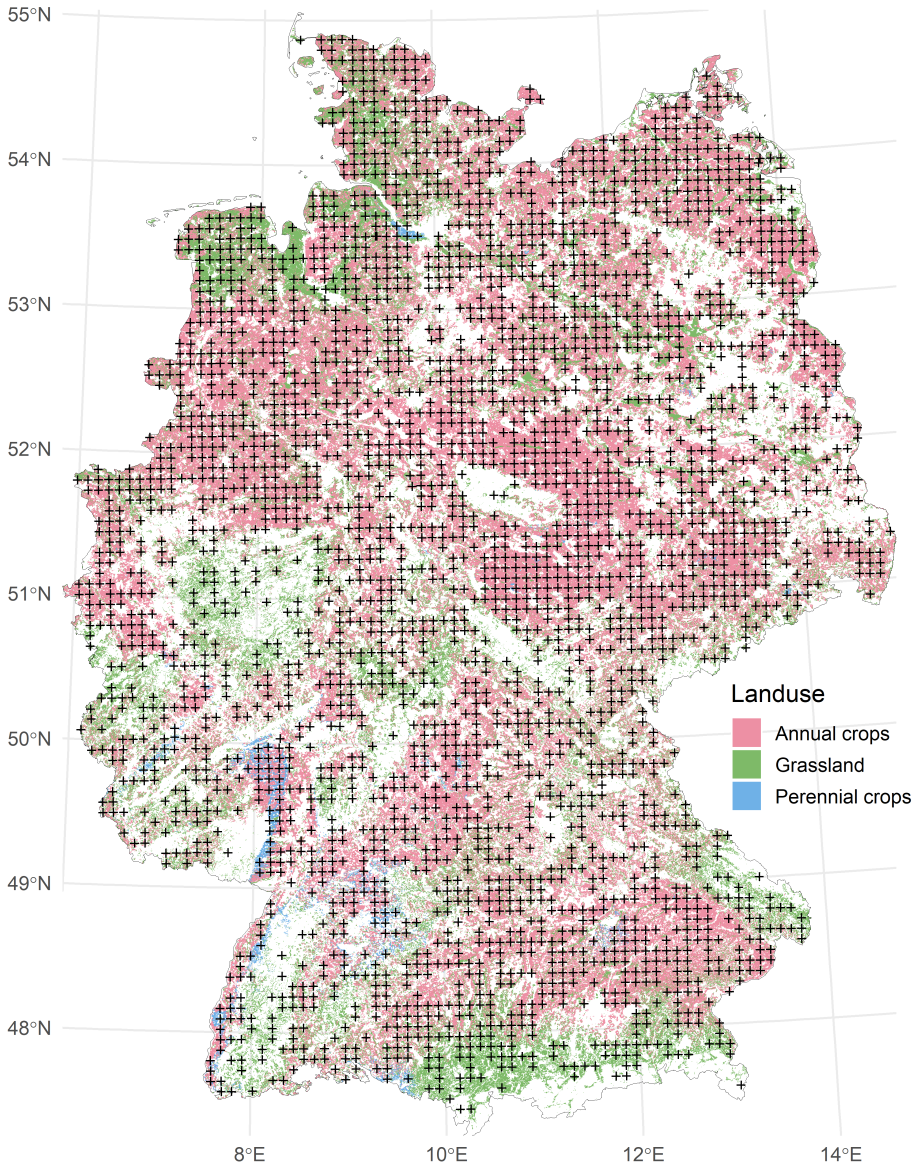


Figure 1.1: Sampling grid of the German Agricultural Soil Inventory (plus symbols). Background map illustrates the total spatial extent of agricultural soils in Germany (BKG, 2020).

1.4 The data-driven approach

In this thesis, data-driven modelling, commonly referred to as machine learning, was used to better exploit the wealth of data provided by the recently completed German Agricultural Soil Inventory. Specifically, this was the case for quantifying traffic induced soil compaction (chapter 2), for unravelling associations of soil organic C with pedology, geology, climate, landuse and management data (chapter 3), and for identifying regional patterns in the melioration of RRLs (chapter 4).
Often, machine learning is regarded as an obscure “black-box” technology. However, in recent years, great efforts have been made to render machine learning more interpretable (Molnar, 2019) and the contribution of machine learning to scientific advance – as promoted by Kell & Oliver (2004) and others – is getting increasingly acknowledged, also in the field of soil science (Padarian et al., 2020). Some machine learning algorithms, including the popular Random Forest algorithm (Breiman, 2001), are actually quite interpretable by design. Apart from its interpretability, the popularity of the Random Forest algorithm is based on its versatility (target and predictor variables can be continuous or categorical; no/little assumptions about the data), robustness towards over-fitting and outliers, ability to handle “small n large p” problems[4], build-in technology to handle missing observations in predictors, and elegant methods to rank the importance of predictor variables (Hastie et al., 2009; Boulesteix et al., 2012). These characteristics explain why Random Forest was the algorithm of choice for the present thesis. In the following, I will provide a brief overview of the main principles behind the Random Forest algorithm.

1.4.1 How do Random Forest models work?

Random Forests are classification algorithms, which consist of a large number of uncorrelated decision trees. Decision trees split datasets into subsets (nodes) with increasingly homogeneous outcomes. Values of the predictor variables serve as cut-points for the splitting of nodes. The splitting of nodes is commonly referred to as tree-growing. Nodes that are not split further are called terminal or leaf nodes.

[4]Data with low observation numbers (n) and a large number of predictors (p) as well as categorical predictors with a large number of factor levels

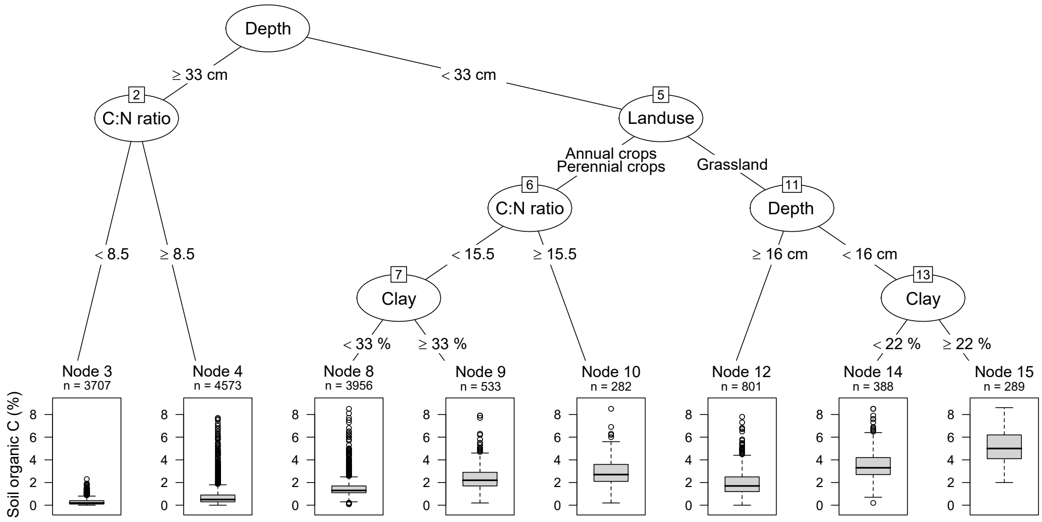


Figure 1.2: Decision tree grown by the CART algorithm to predict the soil organic C content in the upper metre of German agricultural soils from a total of 2931 sites with roughly 5 depth increments each resulting n = 14 529 observations in total.

Various algorithms are available for tree-growing. One of the earliest and still widely utilised is the classification and regression tree (CART) algorithm of Breiman et al. (1984). For predicting a continuous outcome (regression task), the CART algorithm starts by searching every distinct value of every predictor to find the optimum cut-point such that the residual sum of squares (RSS) error in the two resulting daughter nodes N_1 and N_2 is minimised:

$$\mathrm{RSS} = \sum_{i \in N_1} (y_i - \bar{y}_1)^2 + \sum_{i \in N_2} (y_i - \bar{y}_2)^2 \tag{1.1}$$

where $\bar{y}_1$ and $\bar{y}_2$ are the average outcome in the daughter nodes N_1 and N_2, respectively. This minimises the variance within nodes and maximises difference between them. At each daughter node, this procedure is repeated, which recursively partitions the dataset until reaching a pre-defined boundary condition: each partitioning must decrease the overall RSS of the whole tree. Figure 1.2 illustrates an exemplary decision tree grown with the CART algorithm to predict depth profiles of soil organic C content in the upper metre of German agricultural soils. The algorithm was trained using a set of continuous predictors (depth, texture, C:N ratio) and categorical predictors (landuse, WRB soil reference group, groundwater level) with three to eleven factor levels each. The dataset included all mineral soil samples (n = 14 529) of the German Agricultural Soil Inventory. The

algorithm split the dataset first into subsoil (left) and topsoil (right) at a cut-point of 33 cm depth. The depth variable and associated value of 33 cm were chosen because the resulting nodes resulted in a lower RSS (higher difference between nodes) than if any other depth value, texture value, C:N ratio, landuse category, soil group category or groundwater category had served as a cut-point. Subsoil samples (node 2) were subsequently partitioned by C:N ratio. Subsoil samples with C:N ratios < 8.5 (leaf node 3 in the final model), showed significantly lower soil organic C content than other soil samples. Topsoil (node 5), was subsequently partitioned into grassland and annual/perennial cropland because the topsoil of grassland showed much larger soil organic C content than the topsoil of cropland. The recursive partitioning was continued until reaching eight leaf nodes because this is when the algorithm met the pre-defined boundary condition that further splitting always has to improve the overall performance of the whole tree.
In big datasets with many predictor variables of mixed type, complex interactions and non-linear relationships, tree-based models typically outperform classical regression methods with respect to predictive power (Kuhn & Johnson, 2013). Another advantage of tree-based models over linear models is that tree algorithms have build-in technology to deal with missing predictor values (Hastie et al., 2009). In classical regression models, observations with missing predictor values have to be omitted or filled (imputed). Dropping incomplete observations leads to a depletion of the dataset and means that information is lost while the imputation of missing values represents a potential source of bias. Tree-based models can make use of two more elegant ways in dealing with missing predictor values. For one, nodes can be split based on the availability of data (missing vs available). This is relevant if there are systematic differences between complete observations and incomplete observations. For example, if organic soils were included for training the CART algorithm in Fig. 1.2, the algorithm could have used missing texture values to identify soil samples with extremely large soil organic C content. This is because in the dataset of the German Agricultural Soil Inventory, the only soil samples with missing texture values were organic soil samples for which texture was never determined. A second approach, how tree-based models deal with missing predictor values, is the identification of surrogate variables (Kuhn & Johnson, 2013). Surrogate variables provide alternative predictors, which mimic the partitioning of the primary predictor. Surrogate splits make use of the associations among the predictor variables to overcome the problem of missing predictor values. The higher the correlation between two predictors, the lower the loss of predictive

power if one of the predictors contains missing values (Hastie et al., 2009). For example, if the dataset used in Fig. 1.2 showed missing C:N values, at node 2, the soil reference group would have served as the first surrogate (alternative) predictor. This is because the algorithm observed that, at this node, soil groups could produce a similar splitting pattern as achieved by the primary predictor (C:N ratio). Subsoil samples with missing C:N values from Cambisols, Luvisols, Regosols or Stagnosols would have been automatically sent down to the left leaf node, i.e., mimicking C:N ratios < 8.5, while soil samples from all other soil groups would have been sent down to the right leaf node.

Single decision trees are easily interpretable and provide a nice tool for discovering rough data patterns. Also single decision trees provide simple estimates for outcomes. However, minor changes in the training data can result in very different tree structures, and, for regression tasks, the lacking smoothness of single decision trees degrades model performance (Hastie et al., 2009). Random Forest algorithms overcome these drawbacks by generating a large number of different decision trees that operate as an ensemble instead of basing the final prediction on a single model (Breiman, 2001). The number and diversity of decision trees attributes Random Forest algorithms much better predictive performance than what could be achieved by single trees (Liaw & Wiener, 2002). In Random Forests, diversification is achieved by building trees from random subsets of the original dataset. For one, random subsets are formed by bootstrapped resampling of observations. When applying the Random Forest algorithm in practice, 50 to 1000 trees are typically grown from bootstrapped resamples. The aggregation of these individual trees, commonly referred to as “bagging”, smoothens the predictions from individual trees. This can be visualised best with the help of very simple models that use only one predictor as in the example of Fig. 1.3. The strength of tree-based algorithms, however, lies in tasks that involve a large number of predictors. In the presence of many different predictor variables, Random Forest algorithms do not only apply bootstrapped resampling to diversify the trees. In order to reduce the correlation amongst individual trees further, at each split, Random Forests search only in a randomly chosen subsets of the predictor variables for optimal cut-points. For example, instead of considering depth, texture, C:N ratio, landuse, soil group and groundwater level for predicting soil organic C content, Random Forest might consider C:N ratio, landuse and groundwater level for the first split, and depth, texture and soil group for the second split etc. At a first glance, the “mess” achieved by bagging and subsetting of predictor variables might seem

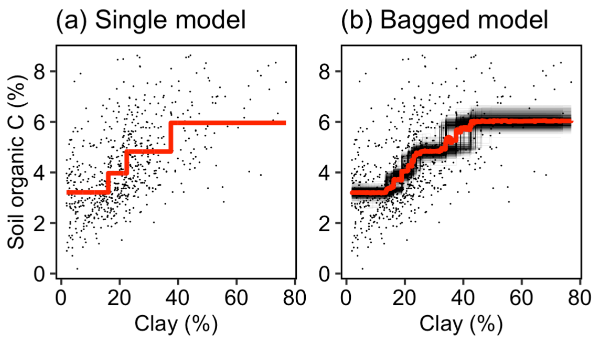


Figure 1.3: Soil organic C content in the upper 16.5 cm under grassland (corresponds to node 13 in Fig. 1.2) as a function of clay content. Predictions derived with decision trees. Left: result based on a single decision tree grown from the entire dataset (red line). Right: result from individual trees (black lines) grown from n = 1000 bootstrapped resamples of the dataset and the result for the corresponding bagged ensemble (red line).

counter intuitive. However, it is exactly the large number of diversity of trees what attributes Random Forest its high predictive strength (Liaw & Wiener, 2002).

1.4.2 How can Random Forests models be used to unravel unknown data patterns?

In the present thesis, the predictive power of Random Forests was used to infer depth profiles of soil compactness and to quantify traffic induced soil compaction (chapter 2). However, the main area of application for Random Forests went beyond mere prediction and Random Forest models were used to characterise associations between predictor variables and given targets. This was achieved by first training Random Forest models and then ranking the importance of all predictors. The importance of a predictor was evaluated by measuring the increase in model error after permuting (deleting the information of) each predictor one at a time. First introduced by Breiman (2001), the concept of calculating permutation importance has been gaining large popularity and, today, it represents a standard method in machine learning (Fisher et al., 2019). Applying Random Forest on the soil organic C example from above (Fig. 1.2), the algorithm identified significant differences in the importance of predictors (Fig. 1.4). Permuting the depth variable increased the mean square error (MSE) by more than 200 %. This was a larger increase in model error than what was observed for permuting any of the other predictors. Therefore, the depth variable was ranked as most important for predicting soil organic C content. In order to make the variable importance measures better comparable, "relative importances" are often reported (Kuhn & Johnson, 2013). Relative importance simply refers to reprojected MSE values such that their cumulative sum gives 100. This reporting style was adopted in the present thesis (Fig. 2.7, Fig. 3.2, Fig. 4.4, Fig. 4.6).

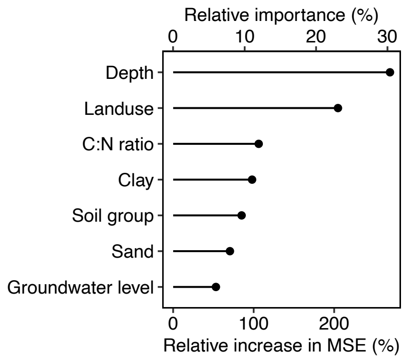


Figure 1.4: Variable importance for predicting soil organic C content using a Random Forest model consisting of n = 1000 trees. Importance is expressed once as the relative increase in the mean square error (MSE) after permuting each predictor (bottom axis) and as relative importances (top axis).

Chapter 2

Extent and cause

Adapted from
Schneider, F. & Don, A. (2019). Root-restricting layers in German agricultural soils. Part I: Extent and cause. Plant and Soil, 442(1):433-51.

2.1 Introduction

Root-restricting soil layers (RRLs) pose a barrier to vertical root elongation, which can severely hamper the production capacity of agricultural land. Barriers for root elongation can make cultivated plants more susceptible to drought (limited nutrient and water acquisition) and toppling (reduced anchorage) or cause stunted growth in sugar beet (*Beta vulgaris* L.) and other root/tuber crops.
In soil without RRLs, subsoil resources have been shown to be of great importance for crop productivity: plant-available water stored in the subsoil can mitigate drought stress long after topsoils have dried out (Barraclough et al., 1989; Kirkegaard et al., 2007). Subsoils also store nutrients that may contribute to plant nutrition (Kautz et al., 2013). This is especially true for mobile nutrients such as nitrate, which quickly leach below the topsoil after applications of mineral fertiliser or mineralisation of organic matter (Dunbabin et al., 2003; Lynch et al., 2012). For loess soils in central Germany, Kuhlmann et al. (1989) documented that up to 75 % of total nitrogen uptake in winter wheat (*Triticum aestivum* L.) is derived from the subsoil. Subsoil resources can buffer yield losses if topsoil resources are temporarily or chronically not available. Thus the importance of accessible subsoil water and nutrients to plant nutrition is elevated during droughts (Kirkegaard et al., 2007; Lynch, 2013) and in low-input cropping systems (Kuhlmann & Baumgärtel, 1991). RRLs render these additional water and nutrient resources unavailable.

In temperate agro-ecosystems, rootability, i.e., the potential of roots to elongate in soil, is often physically and/or chemically constrained (Jin et al., 2017; Lynch & Wojciechowski, 2015). For example, acidity and waterlogging-induced anoxia can severely hamper root growth. Apart from these chemical restrictions to root growth, rock fragments impose a common physical obstacle for root elongation of annual plants (Kutschera et al., 2009). Rock fragments force plant roots to adopt circuitous vertical growth, and thus incur higher metabolic costs in reaching subsoil resources compared to sites with fine soil only. Babalola & Lal (1977) estimated that the negative effects of rock fragments on root elongation outweigh the positive effects of gravel content, such as enhanced water infiltration and aeration, if the gravel content is above 10-20 vol-%. Valentine et al. (2012) proposed soil strength to be the dominant limitation for root elongation in UK agricultural soils. Soil strength, which is sometimes also called mechanical impedance, characterises the resistance of the soil matrix against deformation (Lynch et al., 2012). Fusing of soil particles, for example with silica, iron oxides or calcium carbonate, can lead to cemented pans during pedogenesis (van Breemen & Buurman, 1998). Such cemented pans exhibit high soil strength and therefore restrict rooting into the subsoil. In unconsolidated soil, soil strength largely depends on bulk density, texture and water content. Bulk density and texture can be used to calculate packing density (PD), which describes the apparent compactness of soils better than bulk density alone (Daddow & Warrington, 1983; Huber et al., 2008; Jones, 1983; Renger, 1974). Increasing PD retards root growth (Tardieu, 1994), although some roots might still be able to penetrate densely packed soil by elongating through structural cracks and biopores (Stirzaker et al., 1996). Seasonal changes in soil water content also exhibit a great influence on soil strength. Dry soils tend to be hard because capillary bridges between soil particles induce tensile forces (Bengough et al., 2011; Kolb et al., 2017; Lynch et al., 2012). This explains why soil strength can change drastically across both space and time. In coarse-textured subsoils, however, the influence of water on soil strength seems less important. Here, sand particles tend to be rigidly embedded and interlocked, which induces a high soil strength despite relatively high macroporosity (Lipiec et al., 2016). The interlocked bedding of rough sand grains may explain the commonly observed shallower rooting depths in coarse sandy compared to loamy soils (Batey & McKenzie, 2006; Cruse et al., 1980; Lipiec et al., 2016; Madsen, 1985).

Apart from pedogenic and geogenic causes, RRLs can also form due to agricultural management. Numerous studies assume that the soil strength of central European cropland has increased in recent decades because of traffic-induced soil compaction (Håkansson & Reeder, 1994; van Ouwerkerk & Soane, 1994). This assumption is supported by significant increases in the weight of farm machinery during the past decades. For example, Schjønning et al. (2015) estimated the weight of fully loaded combine harvesters to have increased about sixfold, from 4 Mg in 1958 to 25 Mg in 2009. Also, direct wheeling on top of the subsoil during ploughing operations has been identified as a particularly harmful management practice because compacted subsoil is beyond the reach of annual mechanical loosening operations (tillage). Nevertheless, such in-furrow ploughing has been common practice during ploughing operations all over central Europe. In the early 1990s, Oldeman et al. (1991) estimated that 33 million ha of agricultural land in Europe was degraded because of traffic and ploughing-induced soil compaction. This corresponds to about 4 % of total agricultural land. In Germany, about 10–20 % of cropland has recently been classified as anthropogenically compacted, based on expert judgments (UBA, 2018). However, data availability to quantify the extent of compacted subsoils beyond field scale has been scarce, and therefore the numbers quoted above are highly debated (Vorderbrügge & Brunotte, 2011). The controversy in quantifying the regional extent of compacted farmland revolves around the choice of appropriate indicators and threshold values to demarcate compacted from non-compacted soil, and the representativeness of available measurements for the region of interest. In the past few decades, new agricultural technologies have emerged that help to prevent soil compaction despite high wheel loads, e.g., automatic tyre pressure control systems and out-furrow ploughing (Chamen et al., 2003; Tullberg, 2018). Furthermore, farmers' awareness of compaction has risen and many farmers who are aware of the compaction problem avoid trafficking wet soil today (Batey, 2009). Thus, the extent of compacted European cropland today is still unknown.

In Germany, 70.6 % of agricultural land is used for annual crops, 28.1 % for permanent grassland and 1.2 % for perennial crops such as vineyards (Destatis, 2019). Only about 3 % of agricultural land is irrigated (Destatis, 2017b). Thus the vast majority of farmers is rainfed. Annual crops are dominated by winter wheat, with 25 % of cropland cultivation. In recent decades, dry spells have caused increasingly severe yield losses in winter wheat (Lüttger & Feike, 2018). In 2018, yield losses due to drought were particularly pronounced, with the yield of winter wheat growing in northeast Germany 26 % lower than the decadal average (Statistisches

Amt Mecklenburg-Vorpommern, 2018). In the future, dry spells are likely to be amplified due to greenhouse gas-induced global warming (Pfeifer et al., 2015). Thus deep rootability and the associated availability of subsoil water will be of increased importance in mitigating drought stress. However, little is known about the extent of RRLs in Germany. The present study used the first German Agricultural Soil Inventory to examine soil compactness and other RRLs at national scale. Specifically, the objectives of this study were:

- to characterise the extent and distribution of RRLs in agricultural land in Germany
- to estimate their effect on root growth and crop yield, and
- to quantify the effect of land use and management on soil compactness.

2.2 Materials & Methods

2.2.1 The German Agricultural Soil Inventory

The dataset of the first German Agricultural Soil Inventory (2011–2018) comprises soil, management and yield data from 3078 sites covering all cropland and cultivated grasslands of Germany in a grid of 8 km x 8 km (Jacobs et al., 2018). At each site, soil profiles were dug down to 100 cm depth and soil morphology was characterised in accordance with AD-HOC-AG Boden (2005) for each soil horizon. Soil samples were taken at fixed depth intervals (0–10, 10–30, 30–50, 50–70 and 70–100 cm). If soil horizons changed between depth intervals ($>$ 5 cm above or below sampling thresholds), additional samples were taken in order to match each soil sample with the corresponding soil horizon. All soil samples were analysed for texture, bulk density, soil organic carbon (SOC), inorganic carbon, pH (1:5 in water) and other physicochemical soil properties (Table A.1; (Jacobs et al., 2018)). In all, data from 15 125 soil horizons and 16 778 soil samples were evaluated for this study. All soil analyses were conducted in the same laboratory and all soil horizons were characterised by well-trained experts (eight experts covered 89 % of all sites). Information on crop rotations, yields and management was derived from farmer questionnaires (Table A.1).

2.2.2 Definition of root-restricting soil layers

The literature was reviewed for soil parameters that have previously been shown to restrict root growth on agricultural land in a temperate climate. The search resulted in a total of seven parameters (Table 2.1, Fig. A.1). For each parameter, the literature was screened for threshold values beyond which root growth was restricted. If this threshold was unambiguous (e.g., bedrock: no/yes), two levels of root restriction were defined: no root restriction (e.g., bedrock: no) and severe root restriction (e.g., bedrock: yes). If reported threshold values differed, three levels of root restriction were defined: soil layers with parameter values beyond the most extreme threshold value were classified as severely root-restricting, soil layers with parameter values between the least and most extreme reported threshold values were classified as moderately root-restricting, and the remaining soil layers with parameter values below the lowest threshold value were classified as not root-restricting, i.e., lower than moderate or severe root-restriction. Discretizing the degree of root restriction was a necessary simplification because, to the best of our knowledge, no function exists that relates soil properties to root restriction at continuous scale and under field conditions. Restricted root elongation due to compactness was evaluated on the basis of PD – a parameter which is in good agreement with other common indices describing the compactness of soils, such as least limiting water range (Da Silva & Kay, 1997; Kaufmann et al., 2010), S-Index (Dexter, 2004; Kaufmann et al., 2010) and degree of compactness (Naderi-Boldaji & Keller, 2016, Fig. A.2). PD was calculated after Renger et al. (2014):

$$PD = Bulk\ density + 0.005 * clay + 0.001 * silt \tag{2.1}$$

where both PD and $Bulk\ density$ are given in $\mathrm{g\,cm^{-3}}$, and $clay$ and $silt$ contents are given in mass-%. $Bulkdensity$ refers to the dry bulk density of fine soil (< 2 mm) and was calculated as $(m_{tot} - m_{coarse} - m_{roots})/(V_{tot} - m_{coarse}/\rho_{coarse} - m_{roots}/\rho_{roots})$ where V_{tot} is the volume of an undisturbed soil core in $\mathrm{cm^{-3}}$, m_{tot} is its corresponding mass in g after drying at 105 °C) until constant weight, m_coarse is the dry mass of the coarse fraction > 2 mm in g, ρ_coarse is the density of the coarse fraction in $\mathrm{g\,cm^{-3}}$, m_{roots} is the dry root mass, and ρ_{roots} is the density of roots which was assumed to be $1.0\,\mathrm{g\,cm^{-3}}$ (Barber, 1995). If field workers estimated ρ_{coarse} to deviate from normal ($2.65\,\mathrm{g\,cm^{-3}}$), ρ_{coarse} was determined in the laboratory with a particle density determination kit (YDK01, SARTORIUS). Soil cores were usually obtained using sample rings on profile walls. In a few cases, the soil cores were taken with a driving hammer (Walter et al., 2016). Soil texture was measured by sedimentation/pipette method for 97 % of all samples. For the remaining samples, texture was inferred from NIR spectra following Jaconi et al. (2019b). Reported threshold values for restricted root growth due to high PD differed. The upper threshold value ($1.82\,g\,cm^{-3}$) was extracted from Kaufmann et al. (2010) while the lower value ($1.75\,g\,cm^{-3}$) was based on Huber et al. (2008). Bedrock was defined as consolidated rock that is not diggable with a spade. Bedrock is widely agreed to restrict root growth and is therefore classified as restricting root growth severely (Schoeneberger et al., 2017). Rock fragment content was determined following the standard procedures of German soil inventories in forestry (GAFA, 2014). The content of gravel sized rock fragments (in vol-%) was calculated as m_{gravel}/ρ_{gravel}. The volumetric fraction of cobbles, stones and boulders was estimated directly in the field and added to the volumetric fraction of gravel. In the literature, reported rock fragment contents beyond which root growth was restricted differed. The most extreme threshold value (88 vol.-%) was based on Leenaars et al. (2018), while the least extreme threshold value (75 vol.-%) was extracted from Stahr et al. (2016). Cementation was characterised based on the German classification system for soil horizons (AD-HOC-AG Boden, 2005). As per the definition, horizons classified as “m” describe strongly cemented soil layers such as hard iron pans in Podzols, while cemented soil structure (“Kittgefüge”) also includes moderate degrees of cementation (e.g., friable iron pans). Therefore, all soil horizons encoded with “m” were classified as severely root-restricting, and all soil layers with a cemented soil structure but without horizon code “m” were classified as moderately root-restricting. Inclusion of sandy subsoil as an indicator of restricted root growth was inconsistent in the literature. For example, the USDA Soil Survey Handbook (Soil Science Division Staff, 2017) does not include sandy subsoils as a standalone criteria for restricting root growth, while other handbooks (Müller et al., 2007) and reviews (Batey & McKenzie, 2006) do. Due to the inconsistent reporting in the literature, sandy subsoils were assumed to restrict root growth only moderately. The corresponding threshold value (95 %) was extracted from Leenaars et al. (2018). Owing to ambiguous findings for topsoils (Poeplau & Kätterer, 2017), soil layers with $> 95\,\%$ sand were only classified as moderately root-restricting at $> 30\,cm$ depth. The degree of anoxia was characterised by visual examinations of soil profiles after AD-HOC-AG Boden (2005). Soil horizons, in which reducing conditions occurred on roughly > 300 days per year, were classified as anoxic (pedogenic horizon code “r”). In the literature, anoxia is widely agreed upon as restricting root growth (Soil Science Division Staff, 2017). Therefore, anoxic soil layers were classified as restricting root growth severely. Acidity was inferred from pH measurements in double deionised water (5 ml soil in 25 ml water). The reported pH values beyond which root growth was restricted differed. The lowest value (pH 4) was based on Slattery et al. (1999) and the upper value (pH 5) on Lynch & Wojciechowski (2015).

2.2.3 Effect of root-restricting layers on root distribution

The effect of moderate and severe RRLs on subsoil rooting was quantified using root counts from profile walls (Fig. A.3). Root counts were originally given in ordinal classes for fine, coarse and unspecified-sized roots (AD-HOC-AG Boden, 2005). These classes were converted to a numeric scale based on Table A.2 and the numbers summed to yield root counts per dm^2 and soil layer (independent of root size). Root counts from sites (i) without any variation along depth, (ii) with fewer than 4 roots dm−2 in 0–10 cm, or (iii) with increasing root counts with depth were omitted in order to increase the comparability between sites. As root counts were available only once per site at the time of soil sampling, they referred to different plants (species and cultivars), growing stages, management and growing seasons (weather conditions). This induced considerable variation in the root count data, which was not related to RRLs. In order to still see the effects of RRLs on subsoil rooting, this study (i) restricted the evaluation to roots in permanent grassland and roots of winter wheat (most common crop type), (ii) evaluated all RRLs combined and only the most common cause of root restriction individually (compactness), and (iii) normalised the observed root counts for each site by dividing the root count at a given depth by the root count of the uppermost soil layer (0–10 cm). These normalised root counts are referred to below as relative root counts. Basing the analyses on relative instead of absolute root counts increased the comparability of root data between sites. Sites with RRLs in 0–10 cm depth (5 % of all remaining sites) were excluded from the analysis. The relationship between RRLs and relative root counts was examined by depth (30–50 cm, 50–70 cm and 70–100 cm). This was not done for 10–30 cm because of the low number of sites with RRLs at this depth . A given site was classified as root-restricting at $depth_i$ if root restriction occurred at or above $depth_i$. This was done in order to account for the fact that RRLs (e.g., severely compacted plough pan at 30–50 cm) act as a barrier to vertical root elongation into greater depths (e.g., subsoil below the plough pan).

2.2.4 Effect of root-restricting layers on crop yield

In order to discuss the severity of RRLs, grain yields of winter wheat were compared at sites with and without RRLs in 0–100 cm depth. Winter wheat was selected because this was the most common crop. The comparison was based on multi-annual average yields per site. Only sites with yield data of two or more growing seasons were included (87 % of total cropland). The yield data were derived from farmer questionnaires on crop yields of the sampling sites in the 10 years prior to sampling. Crop yields were compared for all RRLs combined and for compactness, which was the most common RRL on sites used for winter wheat. Yield effects due to compactness were additionally evaluated based on a drought index. If cumulative daily precipitation from April to June (DWD, 2019b) was below median average (171 mm), the growing season was classified as “dry” and if it was above that value as “wet”.

2.2.5 Causes of soil compactness

The main drivers of the compactness (PD) of German agricultural soils were identified using Random Forest models on each land use (only annual crops, only grassland or all land uses with land use as a predictor variable) and depth category (0–10 cm, 10–30 cm, 30–50 cm, 50–70 cm, 70–100 cm or 0–100 cm with soil depth as a predictor variable). Random Forest is presently one of the most successful machine learning algorithms (Biau & Scornet, 2016), which has proven particularly accurate and robust in predicting soil compactness and other soil properties (Hengl et al., 2017). A wide range of pedology, geology, climate and management-related potential predictors of soil compactness were compiled, which partly originated from external sources. A detailed overview of all the input variables is provided in the annex (Table A.1). Since soil compactness does not restrict root growth in peatland and fens, the analyses in this study focused on mineral soils only, i.e., soils containing < 8.7 % SOC (AD-HOC-AG Boden, 2005).

Next, the anthropogenic-induced increase in the compactness of mineral soils under cropland use was quantified. In Germany, most cropland receives frequent trafficking with heavy farm machinery, and links between trafficking intensity and subsoil compactness are frequently reported (Schjønning et al., 2015). Furthermore, cropland contains less SOC than soil under potential natural vegetation such as grassland or forest (Poeplau & Don, 2013), and soil compactness tends to increase with decreasing SOC content (De Vos et al., 2005). However, 93 % of German cropland is regularly ploughed or chiselled (Destatis, 2017a), which loosens the soil structure. Thus, it was assumed that the compactness of cropland (PD_{crop}) can be described as follows:

$$PD_{crop} = PD_{ref} + use + man \tag{2.2}$$

where PD_{ref} is the theoretical, site-specific PD without anthropogenic influence, use describes the land use-induced change in compactness due to SOC losses after conversion to cropland, and man describes management-induced change in compactness due to trafficking/tillage. As grassland is not ploughed (no plough pan) and typically receives a lower trafficking intensity than cropland, it was assumed that

$$PD_{ref} \approx PD_{grass} \tag{2.3}$$

where PD_{grass} is the site-specific PD under permanent grassland use. To quantify man, a Random Forest model was therefore trained only on data from permanent grassland (0–100 cm with soil depth as the predictor variable) and used to predict the PD of cropland as a function of depth ($\widehat{PD}_{crop}$). Only grassland without land use conversions in the previous 30 years was included in the model training in order to omit possible cases of historic plough pans in grassland. If no information on land use history was provided in the farmer questionnaires, sites were only included if soil profiles did not show relic plough horizons. Owing to the nature of available input variables, the grassland model accounted for a wide range of pedogenic, geogenic and SOC (use) effects on PD_{crop}, but was not informed about tillage practices and the hypothesised greater trafficking intensity on cropland (man) compared to grassland:

$$\widehat{PD}_{crop} = PD_{crop} - man \tag{2.4}$$

Rearranging Eq.2.4 gives

$$man = PD_{crop} - \widehat{PD}_{crop} \tag{2.5}$$

Hence, man could be quantified by calculating the residuals of $\widehat{PD}_{crop}$ (Fig.2.1,

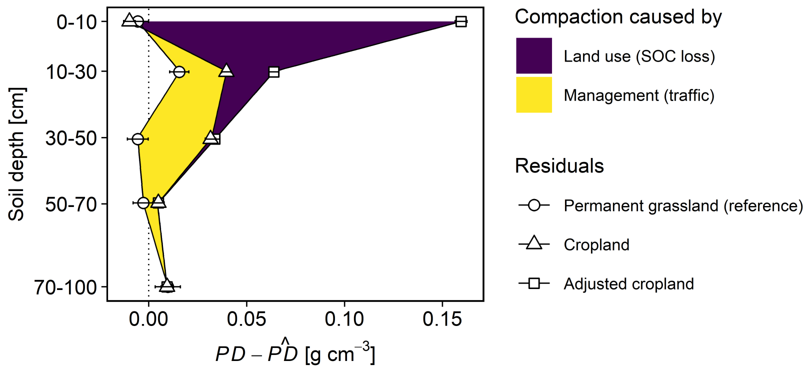


Figure 2.1: Comparison of measured packing densities (PD) and predicted packing densities ($\widehat{PD}$), i.e., residuals, by depth. All predictions were derived from one Random Forest model, which was calibrated only on permanent grassland ($R^2 = 0.77$). For permanent grassland, the out-of-bag residuals were plotted. For cropland, the original dataset (cropland) was used once and a modified dataset with adjusted soil organic carbon (SOC) contents (adjusted cropland) was used once.

triangles). However, the grassland model used to predict $\widehat{PD}_{crop}$ slightly overestimated measured PD in 10–30 cm and 70–100 cm depth (Fig.2.1, circles). Therefore, man was quantified by comparing the residuals of $\widehat{PD}_{crop}$ with the residuals of the out-of-bag estimates for PD in grassland ($PD_{grass} - \widehat{PD}_{grass}$) and Eq.2.5 was corrected accordingly:

$$man = (PD_{crop} - \widehat{PD}_{crop}) - (PD_{grass} - \widehat{PD}_{grass}) \tag{2.6}$$

If the residuals of cropland were higher than in grassland, this was interpreted as increasing compactness due to trafficking (Fig.2.1, yellow area). In order to quantify use, the site and depth-specific SOC deficit due to cropland use was estimated first. This was done by comparing the SOC contents of cropland and grassland from paired plots, which were examined by Poeplau & Don (2013) in a previous study. In 0–10 cm, 10–30 cm, 30–50 cm and 50–100 cm, grassland had a 2.29, 1.16, 1.03 and 1.00 times higher SOC content respectively compared to soil under cropland use. Thus, the measured SOC contents of cropland in the present study were multiplied by these depth-specific factors and the grassland model run on this adjusted dataset. The resulting predictions ($\widehat{PD}_{adj.crop}$) were assumed to resemble PD_{crop} without tillage, as well as similar trafficking practices (man) and SOC content (use) as in the grassland reference. Thus,

$$\widehat{PD}_{adj.crop} = PD_{crop} - use - man \tag{2.7}$$

Finally, *use* was quantified by merging Eq. 2.5 with Eq. 2.7:

$$use = \widehat{PD}_{crop} - \widehat{PD}_{adj.crop} \tag{2.8}$$
$$= (PD_{crop} - \widehat{PD}_{adj.crop}) - (PD_{crop} - \widehat{PD}_{crop}) \tag{2.9}$$

Thus the change of soil compactness due to SOC loss (*use*) was quantified by comparing the residuals of $\widehat{PD}_{adj.crop}$ with the residuals of $\widehat{PD}_{crop}$ (Fig.2.1, purple area).
The natural (management and land use independent) compactness of a given cropland site i ($PD_{ref,i}$) was calculated as

$$PD_{ref,i} = PD_i - \overline{use} - \overline{man} \tag{2.10}$$

where PD_i represents the measured PD of site i, $\overline{use}$ denotes the average *use*- and $\overline{man}$ the average *man*-effect of all cropland sites. If $PD_{ref,i} > 1.75\,\text{g cm}^{-3}$ (Table 2.1), severe soil compactness was assumed to be of pedogenic or geogenic origin. If $PD_{ref,i} < 1.75\,\text{g cm}^{-3}$ and $PD_{ref,i} + \overline{man} > 1.75\ \text{g cm}^{-3} > 1.75\,\text{g cm}^{-3}$, severe soil compactness was assumed to be management derived (compaction due to tillage/trafficking). If $PD_{ref,i} < 1.75\,\text{g cm}^{-3}$ and $PD_{ref,i} + \overline{use} > 1.75\,\text{g cm}^{-3}$, severe soil compactness was assumed to be land use derived (compaction due to SOC loss). In the following, we define all soil layers with PD above the critical limit of $1.75\,\text{g cm}^{-3}$ as "compacted" (see above) and refer to compression of soil from initially $1.75\,\text{g cm}^{-3}$ to $> 1.75\,\text{g cm}^{-3}$ as "compaction".

2.2.6 Statistics and software

All data analysis was performed using R v 3.5.1 (R Core Team, 2018) in RStudio v 1.1.456 (RStudio Team, 2016). Random Forest models were built as implemented in the randomForestSRC package by Ishwaran & Kogalur (2018). To evaluate the accuracy of Random Forest models, root mean square errors (RMSE) and coefficients of determination (R^2) of out-of-bag estimates were reported, as described by Liaw & Wiener (2002). Variable importance was calculated after Breiman (2001). Those variables with greater importance than expected from a theoretical model in which all variables are equally important were considered influential (Hobley et al., 2015). The effect of influential variables on PD was illustrated in partial dependence plots. This illustrates the relationship between a predictor of interest and PD after adjusting PD for average effects of all other covariates included in the model (Hastie et al., 2009). All figures were created using the ggplot2 package (Wickham, 2016). The same package was used for maps after converting data frames to simple features (Pebesma, 2018). The shapefile of German borders was downloaded from `http://www.bkg.bund.de` (last accessed 29th May). Mean values are represented as mean ± standard error. Mann-Whitney-Wilcoxon tests were used to test whether sample populations were identical. Differences were regarded as significant at p-values < 0.05. If more than two populations were compared, Bonferroni correction was applied.

2.3 Results

2.3.1 Distribution and spatial extent of root-restricting layers

In 71 % of all agricultural soils in Germany, potential rooting was restricted to less than 100 cm depth (Table 2.1; Fig. 2.2). Most RRLs (62 %) were classified as severe barriers to root elongation. Restrictions occurred mainly due to physical soil properties (Fig. 2.3a-e). Moderate and severe soil compactness limited rootability in 46 %, sandy subsoil in 12 %, rock fragments in 8 %, shallow bedrock in 6 % and cemented layers in 2 % of agricultural land. Chemical constraints to root growth occurred in 21 % of all agricultural sites, with high groundwater levels affecting 14 % and acidity 10 % of all sites (Fig. 2.3f-g). Generally, RRLs occurred mostly in subsoils, i.e., in > 30 cm depth, but there was also a considerable number of sites (13 %) with potential limitations to root growth already occurring in topsoils. In cropland, restricted root growth in both the topsoil and subsoil was mostly caused by high compactness. In grassland, acidity was the dominant cause of root restriction in the topsoil, while anoxia was the dominant cause of root restriction in the subsoil due to high groundwater levels.
Compactness increased significantly with soil depth. While in 30–50 cm depth, 20 % of all sites were compacted, this proportion increased to 33 % in 70–100 cm depth. Cropland was more densely packed than grassland (Fig. 2.4). This difference was most pronounced in 0–10 cm and decreased with depth. Sandy subsoil occurred mostly in northwest German lowlands on soils that had developed from Pleistocene sediments (Fig. 2.3e). In the same region, high acidity and, in a few cases, cementation restricted rootability (Fig. 2.3c, g). Most acid soils were either peatland and fens (42 %) or Podzols (20 %). Cementation was mostly of an ortsteinic (83 %) or petrogleyic (6 %) nature. Shallow bedrock frequently occurred

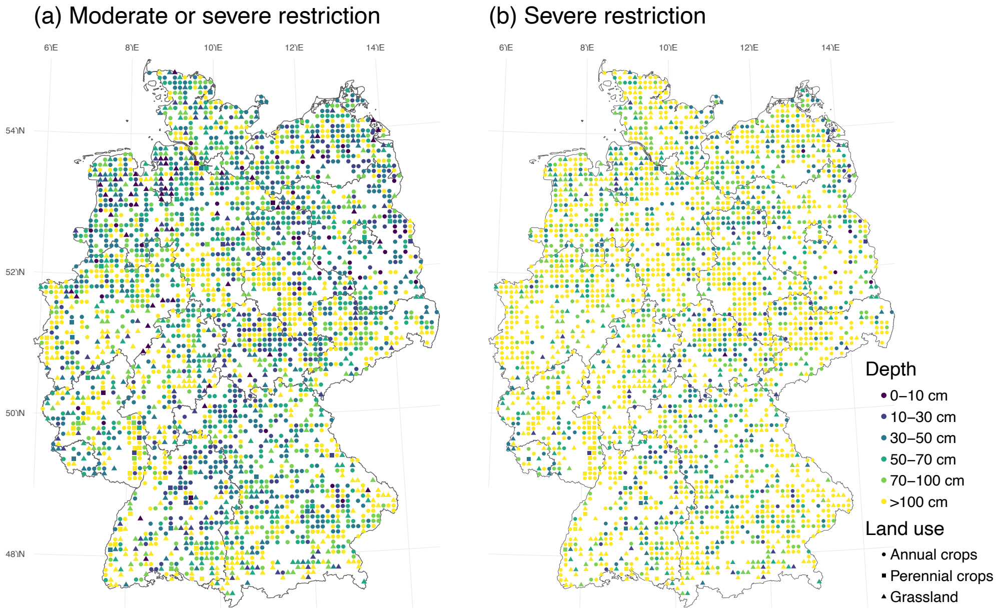


Figure 2.2: Depth to uppermost root-restricting soil layer considering (a) all levels of root restriction and (b) severe root restriction only. Symbol shapes illustrate different land use.

in the peripheral regions of forested lower mountain ranges in central Germany and along the Jurassic in Swabia, southern Germany (Fig. 2.3a). Similar regions were characterised by high rock fragment contents (Fig. 2.3b). Permanent anoxic conditions were a common feature in riverine lowlands (river valleys of the Elbe, Weser and Ems), northwest coastal lowlands and floodplains south of the Danube river (Fig. 2.3f).

2.3.2 Effect of root-restricting layers on root distribution

Relative root counts were significantly lower in the presence of RRLs (Fig. 2.5). This was observed both in cropland with winter wheat (Fig. 2.5a) and in grassland (Fig. 2.5b). The differences were particularly pronounced when comparing relative root counts of severe RRLs to root counts in soil layers without RRLs. In 30–50 cm depth, relative root counts of winter wheat were 18 % lower in the presence of severe RRLs at or above 30–50 cm depth compared to soils without RRLs. In grassland, relative root counts were 32 % lower in the presence of severe RRLs at 30–50 cm depth. Moderate RRLs decreased relative root counts of winter wheat (grassland) by only 10 % (9 %) at 30–50 cm depth (not significant). This confirmed that severe RRLs decreased root elongation more than moderate RRLs.

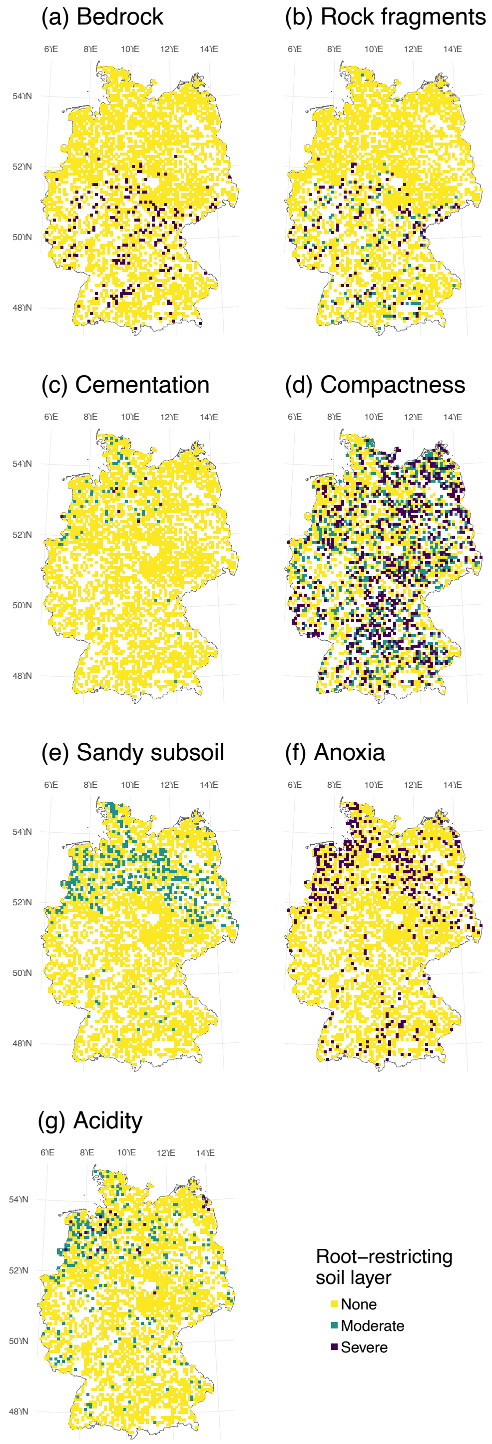


Figure 2.3: Type and magnitude of root-restricting soil layers in $< 100\,\text{cm}$ depth.

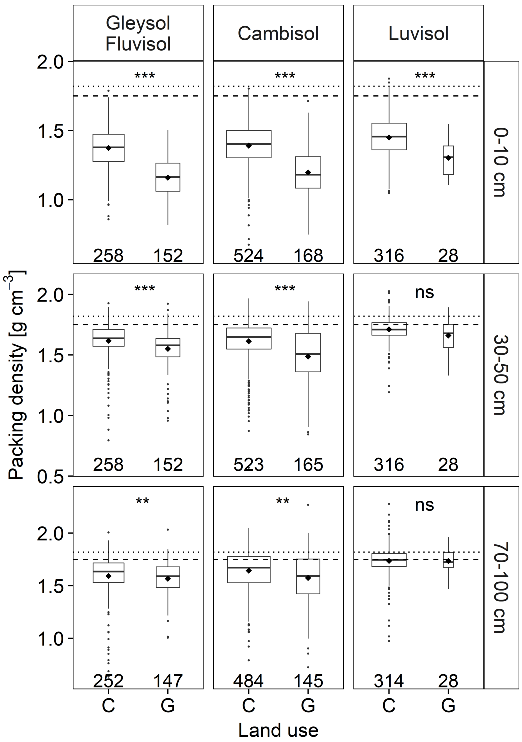


Figure 2.4: Boxplots of packing density for annual crops (C) and grassland (G) by sampling depth and soil type. Only the most common soil types (neglecting Anthrosols) and top, middle and lowest sampling depths are shown. Significance levels are illustrated as ns, *, ** and *** for not significant, $p < 0.05$, $p < 0.01$ and $p < 0.001$ respectively. Boxplot width is proportional to the observation number. Dashed and dotted lines represent moderate and severe threshold values for root restriction respectively.

The observed differences in relative root counts between soil layers without, with moderate and with severe RRLs derived mostly from soil compactness as this was the dominant driver of root restriction in German agricultural soils. At 30–50 cm depth, severe soil compactness (PD $> 1.82\,\mathrm{g\,cm^{-3}}$) decreased relative root counts of winter wheat by 16 % (not significant) and in grassland by 29 % compared to the respective references with low compactness (PD $< 1.75\,\mathrm{g\,cm^{-3}}$).

2.3.3 Effect of root-restricting layers on grain yield of winter wheat

The average grain yield of winter wheat was 6 % lower on sites with severe RRLs compared to reference sites without RRLs. On sites with moderate RRLs, the grain yield of winter wheat was 3 % lower (not significant). When evaluating all causes of RRLs together, differences in grain yield were independent of average soil texture in 0–100 cm (Fig. A.4). However, when evaluating grain yield only

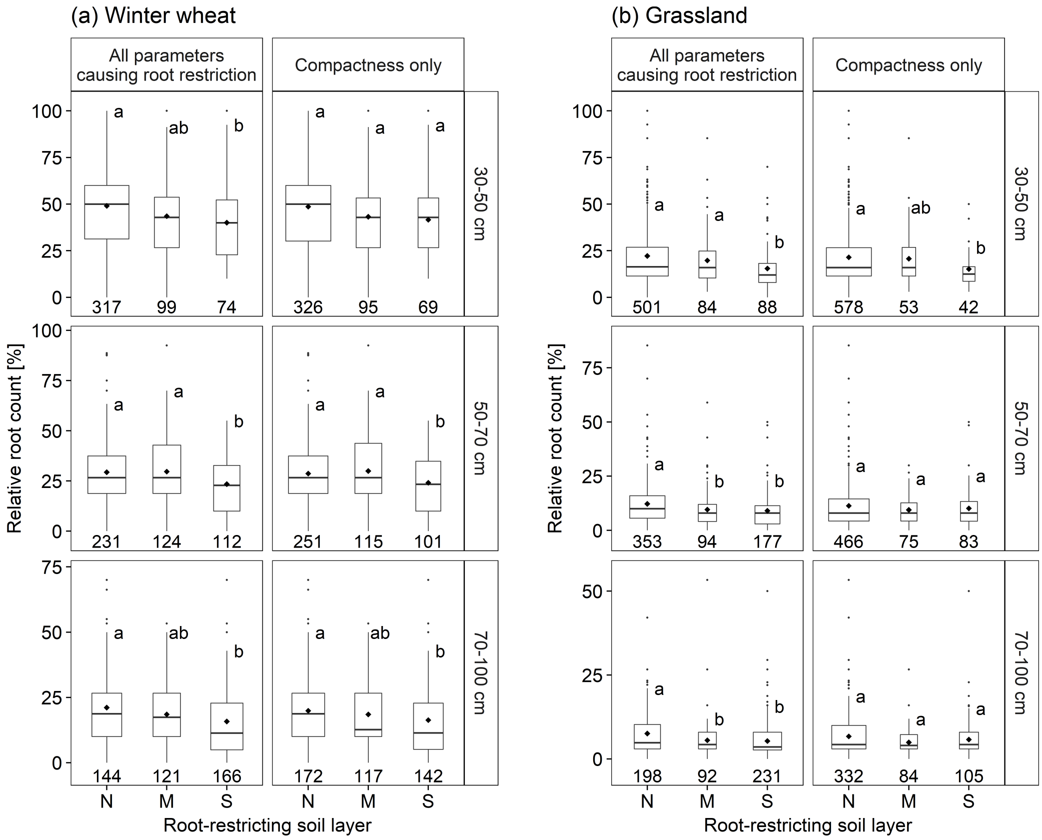


Figure 2.5: Boxplot of relative root counts (root count in 0–10 cm divided by root count at depth$_i$) for no (N), moderate (M) and severe (S) root-restricting soil layers. Root counts sharing the same letter are not significantly different at $p < 0.05$ level. Boxplot width is proportional to the observation number.

with respect to compactness, i.e., neglecting other causes of RRLs, differences in grain yield depended on soil texture: significant differences in grain yield among soils with low, with moderate and with severe degrees of compactness were only observed in soils with a coarse texture (< 17 % clay). Here, severely compacted sites (PD > 1.82 g cm^{-3}) showed 5 % lower grain yields compared to reference sites with low compactness (PD < 1.75 g cm^{-3}). Yield losses on compacted, coarse-textured soil with RRLs were particularly pronounced in relatively dry growing seasons (Fig. 2.6). In relatively wet growing seasons, no significant differences were observed between compacted and non-compacted soil.

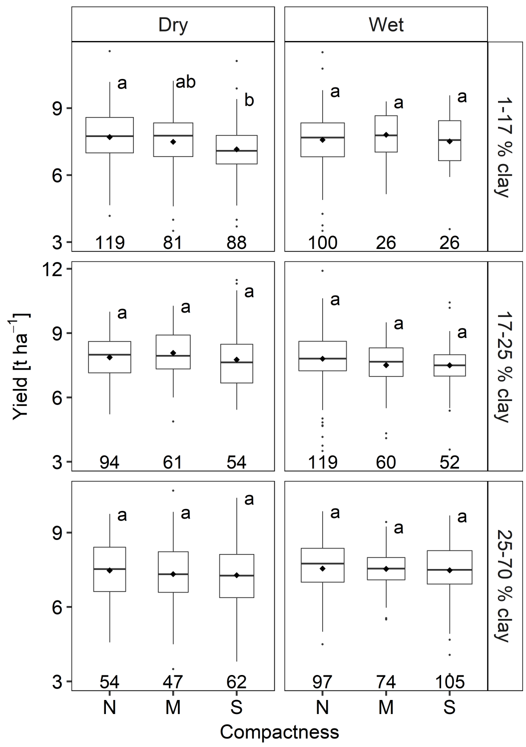


Figure 2.6: Boxplot of grain yield for winter wheat grown on sites with no or low (N), with moderate (M) and with severe (S) compaction stratified by precipitation (columns) and average clay content in 0–100 cm depth (rows). Precipitation was classified as "dry" if cumulative precipitation in April, May and June was below median average (171 mm) and "wet" if it was above that value. Yields sharing the same letter are not significantly different at $p < 0.05$ level. Boxplot width is proportional to the observation number.

2.3.4 Drivers of soil compactness

All Random Forest models predicted PD with high accuracy and R^2 ranging from 0.5 to 0.8 (Fig. 2.7 & Fig. A.5). Only for 0–10 cm in cropland was the accuracy of predicted PD values lower because of limited information on recent tillage practices ($R^2 = 0.3$). Overall, SOC was by far the most important variable for explaining PD (Fig. 2.7). However, the importance of SOC decreased with depth. In grassland, the importance of SOC in explaining PD decreased gradually with depth, while in cropland a sharp decrease was observed between the ploughed horizon and the subsoil below 30 cm (Fig. A.5). Partial dependence plots revealed a strongly negative relationship between PD and SOC, i.e., PD increasing with decreasing SOC (Fig. A.6A). This trend was stronger below 3 % SOC than above this threshold. In the subsoil, the relative importance of rock fragments and texture was similar to that of SOC in explaining PD. Above 5 vol-% rock fragments, PD decreased strongly with increasing rock content, leading to low fine-soil PD in stone-rich soils (Fig. A.6B). Clay was positively correlated with PD (Fig. A.6C). The grassland (reference without anthropogenic increase in compactness) model underestimated measured cropland PD in 10-50 cm depth significantly, suggesting that at this depth increment PD of cropland was increased due to trafficking and tillage (Fig. 2.1, yellow area). This management effect was highest in 30–50 cm depth, where it increased the soil compactness of cropland by on average $0.04 \pm 0.006\,\mathrm{g\,cm^{-3}}$. Additionally, our analysis suggests considerable land use-induced increases in soil compactness due to conversion of natural vegetation to cropland (Fig. 2.1, purple area). Such land use changes decrease the SOC content, which increases PD particularly in 0–10 cm. Cropland soil in 0–10 cm was $0.17 \pm 0.006\,\mathrm{g\,cm^{-3}}$ more densely packed than if the same site were used as grassland. Thus SOC loss increased soil compactness more than traffic. However, in topsoils compactness was mostly far below critical levels. Therefore, SOC loss (land use) pushed only a few sites beyond the chosen critical level of $1.75\,\mathrm{g\,cm^{-3}}$, and traffic (management) was identified as the dominant cause of anthropogenic soil compaction (Fig. 2.8). Overall, the area extent of anthropogenically compacted cropland, where land use and/or management increased the "natural", site-specific packing density PD_{ref} above the chosen critical level of $1.75\,\mathrm{g\,cm^{-3}}$, was estimated to be 13 % (10 % due to traffic, 1 % due to SOC loss, and 2 % due to a combination of traffic and SOC loss). Anthropogenic soil compaction was only detectable above 50 cm depth.

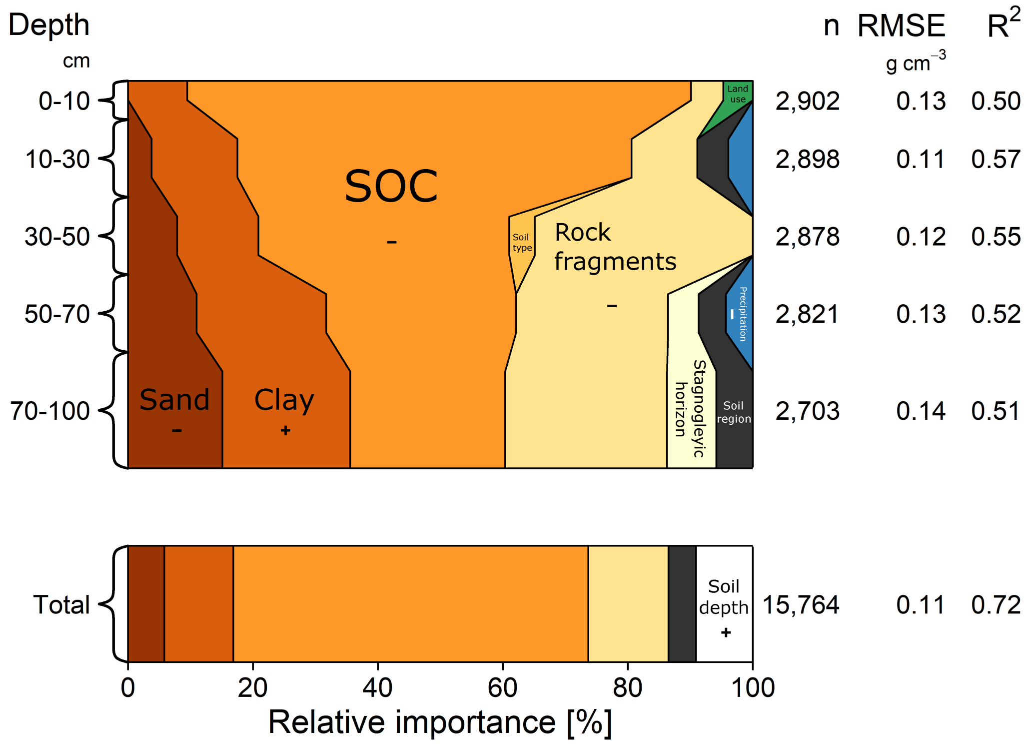


Figure 2.7: Significant predictors of the packing density of mineral soils by depth. Brown and yellow colours represent pedology, grey geology and geomorphology, green represents land use and blue represents climate-related variables. Areas are proportional to the relative importance of the predictors. Each model is characterised by the number of observations in the training data ("n") and errors from out-of-bag data (root mean square error ("RMSE") and R-squared ("R^2")). Positive marginal effects of continuous predictors on packing density are illustrated as "+" and negative effects as "-".

Table 2.1: Potential limitations to root elongation in German agricultural soils at 0–100 cm depth.

Parameter	Description	Threshold values based on literature review		Area extent [%]		
		Moderate barriers	Severe barriers	Moderate barriers	Severe barriers	All** barriers
Physical*				**30**	**32**	**63**
Bedrock	Non diggable, solid bedrock	-	Yes	-	6	6
Rock fragments	All coarse fragments > 2 mm	75-88 vol.-%	> 88 vol.-%	3	5	8
High soil strength						
Cementation	Cemented iron or calcareous hardpans	Cemented structure but no horizon code*** "m"	Pedogenic horizon code*** "m"	2	< 1	2
Compactness	Apparent compactness	1.75-1.82 g cm^{-3}	> 1.82 g cm^{-3}	21	25	46
Sandy subsoil	Interlocked bedding of nearly pure sand in subsoil	> 95 % sand in > 30 cm depth	-	12	-	12
Chemical*				**6**	**14**	**21**
Anoxia	Reducing conditions in > 300 days per year	-	Pedogenic horizon code*** "r"	-	14	14
Acidity	Low pH_{H2O}	4-5	< 4	9	1	10
All parameters*				**27**	**44**	**71**

* At some sites, multiple parameters restricted subsoil rootability, therefore the sum of individual area percentages is greater than aggregated area percentages
** Moderate and severe barriers together
*** Pedogenic horizon codes as defined by AD-HOC-AG Boden (2005), Soil Science Division Staff (2017) and WRB (2014)

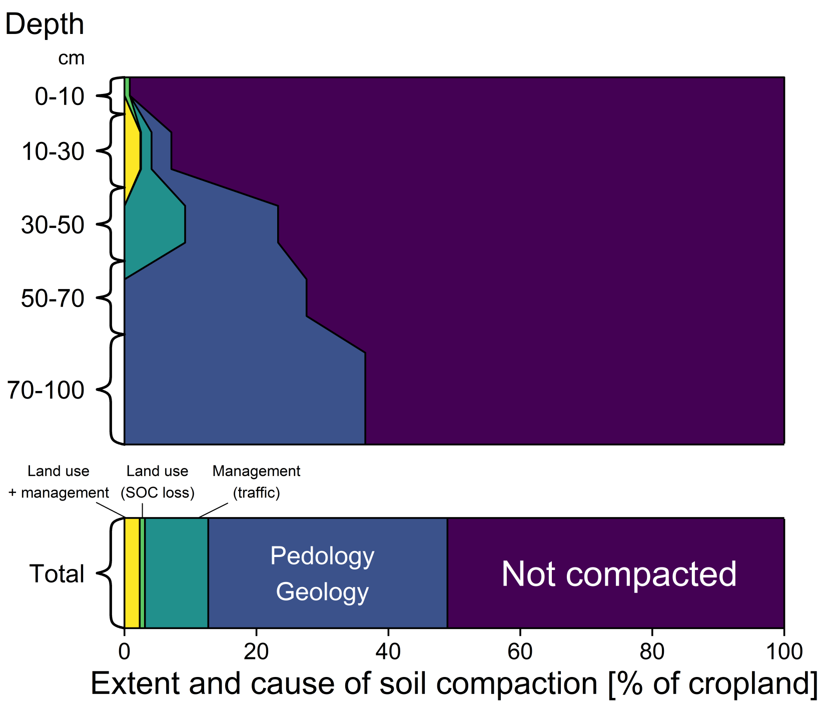


Figure 2.8: Extent and cause of compacted ($> 1.75\,g\,cm^{-3}$) depth increments in mineral soil profiles under cropland use. Anthropogenic soil compaction was separated into land use-induced and/or management-induced compaction. Sites (total) were classified as compacted if they showed at least one compacted soil layer. If there were different causes of soil compaction at a given site (e.g., management in 30–50 cm and pedology in 70–100 cm), only the uppermost compacted soil layer (management) was considered.

2.4 Discussion

The root architecture of cultivated plants is genetically controlled (Lynch & Wojciechowski, 2015), for example dicotyledonous plants such as alfalfa (*Medicago sativa* L.) tend to develop a deeper root system than monocotyledon (Materechera et al., 1992). However, root growth is highly responsive to its environment (Kolb et al., 2017). Therefore, the developmental plasticity of roots is considerable in soils. This has been confirmed in numerous studies (Wasson et al., 2014; Vetter & Scharafat, 1964). It is widely agreed that certain soil properties restrict the root growth of most agricultural plants. However, reported threshold values to distinguish between root-restricting and not root-restricting differ (Table A.1). Based on the range of reported threshold values, soil layers were categorised into non-restricting, moderately root-restricting or severely root-restricting. Using root count data from profile walls, it was possible to validate this concept for winter wheat and grassland by showing significantly different rooting patterns among these three classes. This confirms the direct impact of RRLs on the rooting depth of cultivated crops and grassland species in German agricultural soils.

2.4.1 Natural and anthropogenic causes of restricted rooting

Most RRLs could be attributed to pedogenic and geogenic constraints: rock fragment and sand content are determined by the soil parent material. Furthermore, acid and cemented soil as well as shallow bedrock are primarily of pedogenic or geogenic origin. In some areas, pre-historic land use with heathland might have fostered podsolisation along with acidification and cementation (van Mourik et al., 2012). Historic periods of intense, land use-induced erosion on croplands might also have decreased the soil depth to bedrock (Bork & Lang, 2003). However, the effect of prehistoric land use on present-day RRLs at national scale remains speculative and beyond the scope of this study. Here, the focus was on the role of modern agriculture in forming RRLs. In recent decades, the area extent of RRLs has frequently been assumed to have increased due to management-induced compaction of cropland soils (Schjønning et al., 2015). However a distinction between "natural" (geogenic, pedogenic and pre-historic) drivers of soil compactness and additional compaction by recent cropland use and management has rarely been made due to the methodological challenges this presents. There are three principal options for attributing changes in soil compactness to natural or anthropogenic causes and the most accurate one would be to study the evolution of soil com-

pactness after conversion of natural vegetation to cropland over time. However, a long-term time series of this kind is not available for Germany. Another approach would be to assume that the area extent of naturally compacted land is negligible or confined to certain soil types only. In a recent study, Brus & van den Akker (2018) classified 43 % of the total land area in the Netherlands as compacted. This number was derived from bulk density, texture and SOC measurements directly below the ploughed layer of 128 sites. The authors distinguished between natural and anthropogenic soil compaction based on soil type. The only soil type that was regarded as naturally compacted made up < 1.5 % of the study area Brus & van den Akker (2017), while the remaining, vast majority of compacted land was assumed to be caused by "intensive use of heavy machines".
In the present study, significant effects of soil type on soil compactness were also observed. However, all mineral soil types featured a significant proportion of non-compacted sites. Thus, soil type alone did not suffice to differentiate between naturally compacted soil from anthropogenically compacted soil. Instead, these results suggest that in all soil types, traffic-induced soil compaction (*man*) only acts on top of the natural state of soil compactness (PD_{ref}). This "natural" soil compactness is primarily controlled by SOC and rock content, texture and soil depth (Fig. 2.7). With increasing soil depth, the overburden pressure exerted by the soil column above increases (Gao et al., 2016), while root density and thus SOC content decreases. This explains why most (76 %) compacted sites showed maximum compactness at the maximum sampling depth of 70–100 cm. If soil compaction were mostly caused by traffic, maximum compactness should occur in the uppermost soil layer, which is not being mechanically loosened (tilled) after trafficking, i.e., at 30–50 cm in cropland and 0–10 cm in permanent grassland. However, only 11 % of all the compacted cropland and no compacted grassland showed maximum compactness at these depths. Thus the number of sites that were compacted in close proximity to wheels was much lower than the number of sites that were compacted in deep subsoil layers. This suggests that soil parent material and pedogenesis are important "natural" causes for the observed area extent of compacted agricultural sites. However, the mere comparison of soil compactness by depth did not suffice to quantify the area extent of naturally compacted soil. This was due to the unisotropic nature of agricultural soils. In particular, increasing rock content and buried, relictic topsoil often decreased soil compactness with depth. Therefore, decreasing compactness with depth could not be directly associated with traffic-induced soil compaction. If (i) soil is uni-

sotropic, i.e., under field conditions, and (ii) compactness is not measured before potential anthropogenic compaction occurred, the quantification of anthropogenic compaction is only possible if the compactness of managed sites is compared to the compactness of non-managed reference sites with similar soil and site conditions. This is the third and final approach to differentiate between naturally compacted soil and anthropogenically compacted soil. Typically, such studies are based on a paired plot design in which the compactness of each plot of interest is related to its reference without anthropogenic changes in soil compactness. However, soil inventories, such as that developed in the present study, are not designed in paired plots and the possibilities of construing pairs retrospectively is limited. For example, the present study included far more potentially compacted sites (cropland) than non-compacted reference sites (permanent grassland). Also, average soil and site conditions between cropland and grassland differed (chapter 4). However, grassland sites covered the full range of soil and site properties observed in cropland. Thus, the natural compactness of soil could be modelled based on the soil and site data from permanent grassland. This approach yielded a theoretical, but highly accurate reference for the measured compactness of cropland soil, and finally allowed a differentiation to be made between natural and anthropogenic causes of soil compression (Fig. 2.1). These results illustrate how the anthropogenic influence on soil compactness decreases with depth. Despite tillage (annual loosening), cropland use and management increased the compactness of topsoils by up to $0.17 \pm 0.006\,\mathrm{g\,cm^{-3}}$. This can be attributed to traffic-induced pressure on soil, but also to the SOC deficit of cropland in comparison to potential natural vegetation (Poeplau & Don, 2013). SOC plays a key role in the aggregation of mineral soil particles. SOC loss can therefore cause the collapse of soil structure and soil compression (Soane et al., 1987). However, in the topsoil, compactness was typically far below critical levels for restricting root growth. This explains why, despite the relatively large increases in soil compactness due to recent agricultural practices, only 4 % of cropland was classified as compacted ($\mathrm{PD} > 1.75\,\mathrm{g\,cm^{-3}}$) in the topsoil (Fig. 2.8). In the uppermost subsoil layer directly below the ploughed topsoil, traffic increased the compactness of soil on average by $0.04 \pm 0.006\ \mathrm{g\,cm^{-3}}$. Although the land use and management-induced increase in soil compactness was much lower in the subsoil than in the topsoil, subsoil compression hindered soil functioning more than topsoil compression because the natural compactness of subsoil was closer to the critical level ($\mathrm{PD} = 1.75\,\mathrm{g\,cm^{-3}}$). Small increases in subsoil compactness were often sufficient to push compactness beyond this critical level for root growth. Beyond 50 cm depth, anthropogenic-induced increases in soil compactness decreased to non-significant levels. This is in good agreement with previous findings from controlled field experiments, where various traffic treatments did not compress soil beyond 60 cm depth (Håkansson & Reeder, 1994; Schjønning & Rasmussen, 1994). Traffic-induced soil compression to 90 cm depth as reported by Berisso et al. (2012) could not be confirmed in the present study. Overall, it was estimated that traffic and cropland use-induced SOC-loss together increased the natural compactness of 13 % of German cropland beyond critical limits, i.e., PD $> 1.75\,g\,cm^{-3}$. This area estimate is in perfect agreement with official estimates by the German Environment Agency (UBA, 2018). Based solely on expert judgments, the agency estimates the area extent of anthropogenically compacted cropland to be roughly 10-20 %. In the present study, a novel approach was developed to distinguish between natural and anthropogenic causes of soil compactness in regional soil inventories using machine learning. By adopting this approach in the first German agricultural soil inventory, recent expert judgments on the area extent of anthropogenically compacted cropland with field data could be confirmed.

2.4.2 Effect of root-restricting soil layers on crop yield

In the loess belt and lower Rhine valley, large areas of agricultural land were deep and fertile, with only sporadic occurrences of RRLs (Fig. 2.2). These regions have long been known for their fertility and remain the most productive thus far. In all other regions, physical or chemical barriers for root growth were common features of agricultural land. RRLs limit the availability of nutrient and water resources from deeper soil layers (chapter 5). Experimental field trials from different agro-ecological zones worldwide indicate that limited access to subsoil resources can cause severe yield losses, particularly under drought stress (Kirkegaard et al., 2007). The present study confirms that the adverse effects of RRLs on crop yield are not only detectable in controlled field trials and that they are relevant at national scale: the productivity of agricultural land with RRLs was significantly lower than on land without RRLs. This was despite potential differences in fertilisation, weather conditions, cultivars or pests and diseases, which were assumed to explain the high scatter in the yield data. Negative effects of RRLs on yield of winter wheat were greatest on coarse-textured soils. Coarse soils store less water and nutrients per unit volume than heavy soils. This means plants growing on coarse soils require a larger soil volume to accommodate nutritional needs compared to plants on heavy soil. Crop response to RRLs should thus depend on soil texture and yield losses increase with sand content. The present study confirms this hypothesis (Fig. 2.6). Considering negative yield effects of compaction were only observed under relatively dry growing conditions, highlights the importance of deep water resources for crop resilience. Changing precipitation patterns (Pfeifer et al., 2015) are likely to increase tomorrows importance of subsoil water for plant growth. Thus the observed adverse effects of RRLs on crop yield might intensify in future.

2.4.3 Perspectives

The extent and severity of anthropogenic soil compaction is subject to considerable public debate. For land evaluation purposes, soil compaction is typically evaluated with respect to a critical level of soil compactness beyond which soil functioning is assumed to be significantly constraint. The Joint Research Centre of the European Commission suggested a critical level of $1.75\,\mathrm{g\,cm^{-3}}$ for evaluating the PD of soils (Huber et al., 2008). This threshold value has also been used in the present study to distinguish between compacted (PD $> 1.75\,\mathrm{g\,cm^{-3}}$) and non-compacted soil (PD $\leq 1.75\,\mathrm{g\,cm^{-3}}$). Classifying soil in compacted (restricted root growth) and non-compacted (non-restricted root growth) is a simplification since the response of root elongation to changes in soil compactness can be assumed to be continuous and not discrete. While literature generally confirms the presence of an optimum compactness for root growth and an asymptotical convergence of root growth to zero with increasing compactness (Fig. A.7), defining a threshold value which separates optimum from restricted root growth is arbitrary. For example, choosing a threshold value of $1.82\,\mathrm{g\,cm^{-3}}$ instead of $1.75\,\mathrm{g\,cm^{-3}}$ would have resulted in an area extent of 6 % anthropogenically compacted cropland instead of 13 %. The effect of the chosen threshold value on the area estimates derived in the present study was illustrated in an interactive web-graphic (`https://compact.shinyapps.io/play/`). Arbitrary threshold values call for caution when comparing area estimates on soil compaction from different sources and they explain why any single area estimate on compacted cropland can only be a ballpark figure. For Germany, the present study confirms that anthropogenic compaction poses a significant threat to soil health constraining root growth as well as crop yield at roughly one out of ten unit areas of

cropland. This calls for action. In order to prevent further spread of compacted cropland, farmer extension services and policy makers should continue to promote and support cautious trafficking practices (as little as possible; only when dry; low wheel loads; low tyre pressure; large wheel-soil contact area etc) along with all management practices that enrich SOC contents and prevent erosion of SOC-rich topsoil.
Compacted soil, may it be anthropogenic or pedogenic origin, along with high groundwater levels and soil acidity are the most important causes for restricted root elongation in German agricultural soils. Melioration measures, which improve access to subsoils and their resources could make future farming less vulnerable and more sustainable. By identifying where and why RRLs occur, Part I of this study shows potential target regions for future soil improvement. In Part II, different options for physical, chemical and/or biological soil improvement are discussed (chapter 4).

2.5 Conclusions

The results of this study suggest that 71 % of German agricultural land exhibits barriers for rooting. Most RRLs are of pedogenic and geogenic origin. However, a small, yet significant proportion of RRLs has been caused by human activities: land use and management can increase the compactness of soils beyond critical levels. It is estimated that trafficking, tillage-induced disturbance of soil structure and SOC losses have contributed to compact about one out of ten unit areas of German cropland to an extent that significantly restricts root growth.
Irrespective of their origin, RRLs limit the production capacity of agricultural land. Therefore it is of considerable importance that the further spread of root-restricting, compacted soil layers is prevented. Once they are established, melioration of RRLs is laborious and time-consuming (chapter 4).

Chapter 3

Origin of carbon in agricultural soil profiles

Adapted from
Schneider, F., Amelung, A.,& Don, A. (submitted). Origin of carbon in agricultural soil profiles deduced from depth gradients of C:N ratios, carbon fractions, $\delta^{13}C$ and $\delta^{15}N$. Plant and Soil.

3.1 Introduction

Globally, soils contain about 1500 Pg of carbon bound within soil organic matter in the upper 100 cm (Batjes, 1996). This is about twice the amount of carbon (C) that currently resides in the Earths atmosphere as carbon dioxide (IPCC, 2013). Nevertheless, soil organic C content decreases with greater depth, following the depth distribution of organic C input and its turnover. In agricultural soils, primary organic C inputs may originate from: (i) aboveground biomass that is not harvested, such as stubble, mulch and green manure, (ii) organic fertiliser including animal excreta, compost and biogas digestates, and (iii) root litter and rhizodeposits. The first two sources of organic C enter soil at the surface, with redistribution along the soil profile possibly only occurring via bioturbation, tillage and/or leaching of mobile organic C species. Root-derived C, however, enters soil directly belowground at maximum depths of one metre or more (Canadell et al., 1996). The relative contribution of aboveground biomass, organic fertiliser and roots to total C inputs varies considerably between different land uses and management regimes. Grassland, for instance, receives more C input via roots and rhizodeposits than cropland (Pausch & Kuzyakov, 2018), while cropland receives a larger C input from aboveground in the form of harvest residues and stubble.

After C has entered the soil, it is prone to a range of transformation processes (Kögel-Knabner & Amelung, 2014). Transformation results in significant contributions of microbial debris to total organic C (TOC) (Appuhn & Joergensen, 2006; Liang et al., 2019; Miltner et al., 2012). Microbial transformations of TOC are usually accompanied by stable isotope discrimination processes. Undecomposed photosynthates from annual crops and grasses typically show $\delta^{13}C$ signals from −26 ‰ to −30 ‰ for C_3 plants and −10 ‰ to −14 ‰ for C_4 plants (Philp & Monaco, 2012), as well as $\delta^{15}N$ signals from −8 ‰ to 9 ‰ depending on the nitrogen source (Craine et al., 2015). During microbial processing, the organic C fraction is enriched with heavy isotopes of C and N, which is reflected in increasing $\delta^{13}C$ and $\delta^{15}N$ values (Boutton, 1996b; Natelhoffer & Fry, 1988). If organic material is processed and decomposed, its C:N ratio also decreases from > 15 to the C:N ratio of microbes ranging from 5 to 8 (Amelung et al., 2018). This makes $\delta^{13}C$, $\delta^{15}N$ and C:N values proxies for characterising the degree of microbial processing of organic C and detecting the presence of relatively undecomposed litter. The latter can also be quantified directly by density fractionation, which separates soil organic C into particulate organic C (POC) and mineral-associated C (MOC).

To date, most work on C fractions, $\delta^{13}C$ and $\delta^{15}N$ values, and C:N ratios has rarely gone beyond field scale and has only focused on topsoil because: (i) organic matter in topsoil is more sensitive to land use or management treatments than subsoil, and (ii) measuring and detecting changes in POC, $\delta^{13}C$, $\delta^{15}N$ and C:N signatures of subsoil can be analytically challenging as subsoil typically contains much less organic matter than topsoil. Although globally more than half of the soil organic C in the upper metre is stored below 30 cm depth (Batey & McKenzie, 2006), much less is known about the origin of C in subsoil than in topsoil. Carbon input into subsoils may come from the surface soil and enter subsoil via leaching (Kindler et al., 2011), turbation (bio-, cryo-, or peloturbation), or burial of topsoil C, depending on pedogenesis and climatic regions. However it may also come from the soil parent material, especially if the soil developed from relatively young and C-rich colluvial deposits (Doetterl et al., 2012), or directly from deep roots and their rhizodeposits.

Radiocarbon ages of C in soil profiles suggest that subsoil C-cycling is much slower than topsoil C-cycling. Once C has entered the subsoil, much of it seems to reside there for millennia (Balesdent et al., 1987). Crops deposit about one third of all root C below 30 cm depth (Jackson et al., 1996), but this number varies considerably in time and space. Given the long residence time of subsoil C, increasing root-derived C input in the subsoil on a large scale could remove significant amounts of C from the atmosphere. In this context, the breeding of plants with deep and bushy roots has been proposed as a negative emission technology for counteracting greenhouse gas-induced global warming (Kell, 2011, 2012). However, there are various soil properties that restrict the growth of deep roots, such as compacted soil layers, which are commonly referred to as hardpans (Lynch & Wojciechowski, 2015). Oldeman et al. (1991) projected the global extent of hardpans to be 68 million hectares and attributed hotspots of soil compaction in Europe to heavy machinery. For Germany, (chapter 2) recently estimated half of all cropland to be compacted due to either pedogenetic causes (37 % of cropland) or anthropogenic causes (13 % of cropland). Loosening of these hardpans could promote deep root-derived C inputs and sequester atmospheric C in subsoils.

A better understanding of the origin of C in agricultural soils could improve the design of future climate-smart management practices for enhanced C sequestration. Here, we hypothesised that depth gradients of soil organic C reflect past organic C inputs and allow to track the contribution of deep roots to subsoil C, unless subsoils contain large amounts of topsoil C or parent material-inherent C. We assumed root-derived deep C input to correlate positively with the depth gradients of TOC, C:N and POC:TOC, but negatively with ^{13}C:^{12}C and ^{15}N:^{14}N abundances, as elevated portions of undecomposed root material in the subsoil should also be reflected in lower $\delta^{13}C$ and $\delta^{15}N$ values. We also assumed the depth distribution of root-derived C to be controlled by soil properties and management. We use Germany as a model country, aligning novel data with data from the first German Agricultural Soil Inventory (Poeplau et al., subm) to evaluate the depth distribution of soil organic matter with respect to recent and historic C inputs into agricultural soils at regional scale. Specifically, our aims were to:

- describe the depth gradients of TOC, C:N ratio, POC, $\delta^{13}C$ and $\delta^{15}N$ in the upper metre and relate the observed differences to physico-chemical characteristics of the soil matrix, parent material, climate, land use and/or management using a data-mining approach
- discuss entry pathways and turnover of organic C in topsoils and subsoils
- estimate the effect of hardpans on root-derived C input in subsoil below cropland.

In order to increase the sensitivity of analyses towards site-specific differences in depth profiles, we divided organic C measurements at a given depth_i by the respective organic C measurement of the uppermost sampling layer.

3.2 Materials & Methods

3.2.1 Study area

This study focused on agricultural soils in Germany, which cover an area of 166 451 km^2 (Destatis, 2019). About 70 % of this area is used for annual crops (117 309 km^2), 28 % is used as permanent grassland (47 134 km^2), and the remaining agricultural land is used for perennial crops (Destatis, 2019). Based on FAO (2020), the top three crops grown between 2009 and 2018 were wheat (*Triticum aestivum* L., mean grain yield: 7.6 $Mg\,ha^{-1}$), followed by barley (*Hordeum vulgare* L., mean grain yield 6.5 $Mg\,ha^{-1}$) and canola (*Brassica napus* L., mean grain yield 3.7 $Mg\,ha^{-1}$). German grassland is typically managed intensively and includes 1.4 times more pasture than meadow (Destatis, 2019).

3.2.2 Sampling design & data acquisition

This study was based on the dataset from the first German Agricultural Soil Inventory, which comprises information on the soil and management at 3104 sites covering all agricultural land in Germany in a regular 8 km x 8 km grid (Poeplau et al., subm). At each site, soil profiles were dug to 100 cm depth. Soil morphology was characterised based on soil horizons following AD-HOC-AG Boden (2005), while composite soil samples for laboratory analysis were taken at fixed depth increments (0–10, 10–30, 30–50, 50–70 and 70–100 cm). If a horizon boundary was at least 5 cm above or below a sampling boundary, an additional soil sample was taken. This allowed laboratory and field data to be merged. Total organic C (TOC), total inorganic C (TIC) and total nitrogen were measured by dry combustion using an elemental analyser (LECO TRUMAC, St Joseph, MI, USA). Sand content was determined by wet-sieving, and silt and clay contents following the pipette method. Bulk density, rock fragment fraction and pH_{H_2O} were measured as described by Jacobs et al. (2018).

As processes governing C stabilisation in organic soil differ from those in mineral soils, and as root-derived C inputs contribute only little to C stocks of organic soil, this study focused solely on mineral soils. Therefore, 165 sites with organic soil were removed from subsequent analyses, leaving 15,935 mineral soil samples from 2939 sites for which TOC and C:N values were readily available. For the present study, $\delta^{13}C$ and $\delta^{15}N$ natural abundance as well as C density fractions were also determined. The $\delta^{13}C$ and $\delta^{15}N$ measurements were restricted to 1357 soil samples from 248 core sites. These core sites comprise a representative subset of mineral agricultural soils in Germany with respect to soil reference group, land use and C stock. Detailed criteria for the core site selection are described by Vos et al. (2018). Isotopes were analysed using an isotope-ratio mass spectrometer (IRMS, Thermo Fisher Scientific Delta plus). All $\delta^{13}C$ values refer to the organic C fraction only. Soil samples containing inorganic C were fumigated with hydrochloric acid, as described by Walthert et al. (2010), prior to $\delta^{13}C$ analyses. If total C content based on IRMS was higher than TOC based on dry combustion, inorganic C removal was repeated and $\delta^{13}C$ re-measured. For 183 samples, no reliable $\delta^{13}C$ measurements could be obtained for the organic C, mostly due to incomplete removal of inorganic C at TIC:TOC ratios over 5. Values of $\delta^{15}N$ refer to total N. The $\delta^{13}C$ values are reported relative to Vienna Pee Dee Belemnite and $\delta^{15}N$ values are reported relative to atmospheric nitrogen following international standards.

Particulate organic C to total organic C (POC:TOC) ratios were determined using near-infrared spectroscopy (FT-NIRS; MPA, Bruker Optik GmbH, Ettlingen, Germany). The basic concept for this approach has recently been proven by Jaconi et al. (2019a) who also used soil samples from the German Agricultural Soil Inventory, but focused on topsoil (0–10 cm) only. Here, we present POC:TOC ratios for all depth increments of the German Agricultural Soil Inventory. Our predictions of POC:TOC ratios are based on the same 105 topsoil samples used by Jaconi et al. (2019a), plus additional subsoil samples from 27 of these 105 sites. The 27 subsoil samples were selected to cover the complete range of clay content and C:N ratios of subsoils (Fig. B.1) and were fractionated as described by Jaconi et al. (2019a). However, because the POC content of subsoil was about one order of magnitude lower than in the topsoil, up to 120 g soil instead of 10 g for topsoils were fractionated. This was time-consuming and cost-intensive (up to 620 g sodium polytungstate per sample), therefore not all the sites included in the study of Jaconi et al. (2019a) could be considered for subsoil fractionation. TOC recovery for subsoil samples ranged from 80 % to 120 %. Spectral pre-treatments and models were implemented as proposed by Jaconi et al. (2019a). Additional tree-based model types (ranger, cubist) and modelling approaches (log-ratio transformation of POC and MOC content vs. log-ratio transformation of POC:TOC and POC:MOC, separate prediction of POC and MOC contents vs. separate prediction of POC:TOC and MOC:TOC ratios) were also tested, as detailed in the Supplementary Material B. Model performance was judged based on leave-one-site-out validation. An ensemble of three individual model combinations performed best (Fig. B.2) and was used to predict the POC:TOC ratios of all unseen soil samples.

For the present study, all soil data were aggregated to obtain one single value per depth increment (0–10 cm, 10–30 cm, 30–50 cm, 50–70 cm and 70–100 cm). TOC and TIC concentrations, C:N and POC:TOC ratios, $\delta^{13}C$ and $\delta^{15}N$ values, as well as contents of clay and sand, and pH_{H_2O} values were summarised by weighted means, with fine soil stock of the individual depth increments (Mg soil < 2 mm ha^{-1}) as the weighting factor. For continuous variables given in vol-% (rock fragment fraction) or in area-% (e.g., oximorphic features at the profile wall), the thickness of the respective depth increment served as the weighting factor. Categorical variables with only two levels (e.g., buried topsoil, yes or no) were dummy coded (yes=1, no=0) and also aggregated, with the thickness of the respective depth increment serving as the weighting factor. For categorical variables with more than two levels (soil horizon and stratigraphy), the factor level with the largest contribution to the depth increment was used. Information on crop rotations, tillage and management during the past decade came from farmer questionnaires. Site-specific C input data was estimated by Jacobs et al. (subm).

3.2.3 Analyses of organic C proxies along the soil profile

Each organic C proxy (TOC, C:N, POC:TOC, $\delta^{13}C$ and $\delta^{15}N$) was predicted using machine learning on variables that provided information about current C input (e.g., root-derived C), geogenic C input (e.g., parent material), translocated topsoil C (e.g., horizon symbols), soil transport (e.g., slope) and C stabilisation (e.g., texture). A detailed description of all 39 explanatory variables used is provided in the Supplementary Material (Table B.1, Fig. B.3, Fig. B.4).

In a first step, the machine-learning algorithm was trained to predict the bulk soil value of each organic C proxy (TOC, C:N, POC:TOC, $\delta^{13}C$ and $\delta^{15}N$) at a given depth solely as a function of these 39 explanatory variables. The resulting 25 models (five organic C proxies x five depth increments) were independent of the soil properties in the depth increments above or below. In a second step, tests

were carried out to assess how much and to what depth model performances would improve if the algorithm was also informed about the measured values of the targeted organic C proxy in the uppermost sampling layer. Thus, TOC content from 10 to 100 cm depth was predicted, as was done in the first step, but here included site-specific TOC contents from 0–10 cm depth as an additional (40th) explanatory variable in the models. This was done in an analogous way to also predicting the other organic C proxies (C:N, POC:TOC, $\delta^{13}C$ and $\delta^{15}N$). In the third and final step, the ratio between a given organic C proxy and its value in the uppermost sampling layer (0–10 cm) was predicted. Such ratios are referred to below as "normalised values" to distinguish them from "bulk soil values". Normalised values were used to describe the depth gradients of organic C proxies. For example, if a site showed bulk soil TOC values of 1 g kg^{-1} in 50–70 cm and 5 g kg^{-1} in 0–10 cm, the normalised TOC value in 50–70 cm depth would be 1:5=0.2 or 20 %. Soil layers with normalised values above 300 %, e.g., more than three times as much TOC in 50–70 cm than in 0–10 cm, were treated as outliers and excluded from further analyses. Furthermore, C:N ratios of carbonate-rich soils with more than twice as much TIC as TOC were excluded because these measurements were potentially biased.
For machine learning, the party::cforest implementation of random forest and bagging ensemble algorithms was used (Hothorn et al., 2005; Strobl et al., 2007, 2008) owing to its underlying strength in deriving variable importance from a mix of continuous and categorical predictors (Hapfelmeier et al., 2014). For each model, five folds with three repetitions were applied and the hyperparameter mtry was tuned using grid search on the following values: 3, 6, 13, 26, 39 or 59. The performance of each model was evaluated by root mean square error (RMSE) and mean coefficients of determination (R^2) metrics. Permutation importance was calculated based on Hapfelmeier et al. (2014) using the mtry value that produced the highest R^2. Variables of greater importance than would be expected from a theoretical model where all variables are equally important were considered influential (Hobley et al., 2015). The importance of influential variables was scaled to 100 % for better comparability.

3.2.4 Turnover and mean residence time of organic C

Maize (*Zea mays* L.) was the only C_4 plant in crop rotations, and as such introduced a natural ^{13}C label into the soil. We estimated the fraction F of maize-derived C in TOC after t years of maize based on Balesdent et al. (1987) as:

$$F(t) = \frac{^{13}C_{S1,t} - {}^{13}C_{S0}}{^{13}C_{P1} - {}^{13}C_{P0}} \quad (3.1)$$

where S1 and S0 were the soils of sites with and without maize respectively and P1 and P0 were photosynthates from maize and from other crops respectively. $^{13}C_{P1}$ was set to -12 ‰ (Balesdent et al., 1987). $^{13}C_{S0}$ was defined as the intercept of a linear regression between the number of maize years (t) and the corresponding $\delta^{13}C$ values of soil ($^{13}C_{S1,t}$). The slope of this regression times the number of maize years (t) plus $^{13}C_{S0}$ yielded the $\delta^{13}C$ value of soil after t maize years ($^{13}C_{S1,t}$). The regression was based on 167 cropland sites, for which both $\delta^{13}C$ values and crop rotation data were available. $^{13}C_{P0}$ was assumed to be the same as $^{13}C_{S0}$, which is a common simplification because the difference between C_3 and C_4-derived organic C is typically about one order of magnitude higher than turnover-induced C fractionation in soil (Balesdent et al., 1987; Boutton, 1996b). Crop rotations were reported for 10 years. Potential maize-derived C older than 10 years was assumed to be randomly distributed across sites. Carbon turnover was defined as the average increase in F per maize year.
The mean residence time of organic C was estimated following (Amelung et al., 2018) as $-t/\ln(1 - F(t))$, where $1 - F(t)$ represents the remaining proportion of C_3-C after t years of maize. This approach assumes: (i) TOC stocks to be in equilibrium and (ii) first-order kinetics for organic C decomposition (Balesdent & Mariotti, 1996).

3.2.5 Soil compaction vs. root-derived deep C input

The level of soil compaction was classified according to chapter 2 as not compacted (packing density < 1.75 g cm^{-3}), moderately compacted (1.75 g cm^{-3} $<$ packing density < 1.82 g cm^{-3}) or severely compacted (packing density > 1.82 g cm^{-3}). A given site was classified as compacted at depth$_i$ if a compacted soil layer occurred at or above depth$_i$. This was done in order to account for the fact that compacted soil layers (e.g., ploughpan at 30–50 cm) may act as a barrier to root-derived C inputs at greater depths (e.g., subsoil below ploughpan). Root-derived C inputs were inferred from normalised TOC, C:N, POC:TOC, $\delta^{13}C$ and $\delta^{15}N$ values, i.e., measured values of TOC, C:N, POC:TOC, $\delta^{13}C$ and $\delta^{15}N$ at a given depth$_i$ divided by their respective value in the uppermost sampling layer (0–10 cm). Normalised values were preferred over bulk soil values because normalisation minimised site-specific differences in organic C. The relationship between root-derived C input and soil compaction was examined by depth (30–50 cm, 50–70 cm and 70–100 cm). Topsoil was not considered because the majority of hardpans occurred in subsoils. The analyses were restricted to cropland soil only (2261 sites) because compaction in cropland was more severe than in grassland.

3.2.6 General statistics & software

All data analysis was performed using R (R Core Team, 2019) in RStudio (RStudio Team, 2019) and built on tidyverse packages (Wickham et al., 2019). Computationally intensive code was implemented in parallel using the foreach package (Microsoft & Weston, 2020) and run on a high-performance server with 64 cores (128 threads). Spectral pre-treatments were done using prospectr (Stevens & Ramirez-Lopez, 2013), while pls (Mevik et al., 2019), ranger (Wright & Ziegler, 2015) and cubist (Kuhn & Quinlan, 2018) were used for spectral modelling. Each key statistic in the text is accompanied by its 95 % bias-corrected and accelerated (BCa) confidence interval based on ≥ 3000 bootstrapped resamples calculated using the boot package (Canty & Ripley, 2019).

3.3 Results

Background information on the parameters mentioned in this section can be found in the Supplementary Material B. Table B.1 provides definitions and Fig. B.3 and B.4 illustrate the spatial distribution of the parameters in maps.

3.3.1 TOC

In 0–10 cm depth, TOC content averaged 23.5 g kg^{-1} (95 % CI, 23.0 to 24.1) and its interquartile (middle 50 %) ranged from 12.9 to 29.6 g kg^{-1}. Variation in TOC at this uppermost depth increment was mostly caused by different land use (cropland vs. grassland) and clay content (Fig. 3.1, Fig. 3.2). In 0–10 cm, the TOC content in grassland was 2.4 times (95 % CI, 2.3 to 2.5) greater than that in cropland and increased significantly with clay content (Fig. B.5). Land use and soil texture showed distinct regional patterns, which were reflected in the TOC map (Fig. 3.1): regions with dominant grassland use in south and north-west Germany were associated with elevated TOC values, while large areas with low clay content in north-east Germany showed low TOC values (Fig. B.3, Fig. B.4).

With increasing soil depth, the importance of variables to explain TOC content changed considerably (Fig. 3.2). Instead of land use, climate-related variables were the most important for predicting TOC in 10–30 cm depth. TOC content correlated positively with precipitation and negatively with the number of summer days (Fig. 3.2). The "Weser-Ems-Geest" climatic region in north-west Germany, which is characterised by a maritime climate (high precipitation, not many summer days) and historic heathland and peatland cover, showed the largest TOC content (Fig. 3.3d). In 30–70 cm depth, soil reference group and horizon symbols were most important for explaining TOC. For example, in 50–70 cm, Anthrosols contained 8.4 g kg^{-1} (95 % CI, 7.3 to 9.8), Chernozems, Phaeozems and Vertisols contained 5.8 g TOC kg-1 (95 % CI, 5.5 to 6.2), while all other soil groups contained only 3.1 g TOC kg-1 (95 % CI, 2.9 to 3.2) (Fig. 3.3a, Fig. 3.4). At the same depth, M horizons designating colluvial deposits (mean 7.2 g kg^{-1}; 95 % CI, 6.5 to 8.0) and deep or buried A horizons (mean 5.8 g kg^{-1}; 95 % CI, 4.8 to 7.1) showed significantly larger TOC contents than other soil horizons (mean 3.5 g kg^{-1}; 95 % CI, 3.4 to 3.7) (Fig. 3.3b). Finally, below 70 cm depth, geological chronostratigraphy and texture, both characterising the soil parent material, were the most important for predicting the contents of TOC in this subsoil depth. Holocenic sediments, which comprised mostly fluvial deposits along major river valleys (Elbe and Rhine), marine deposits along the north-west coastline and colluvial deposits at the foot of slopes, showed TOC contents that were three times (95 % CI, 2.6 to 3.4) greater in 70–100 cm depth than soils from other, older parent materials. As with topsoil, the content of clay in subsoil also correlated positively with that of TOC (Fig. B.5). Although TOC content in grassland was significantly higher than that in cropland at all depth increments (Fig. 3.1), land use was not relevant for explaining TOC below 10 cm depth (Fig. 3.2). Different TOC contents in the subsoils of cropland and grassland were related to preferential grassland use on Gleysols, presumably because of traffic restrictions for heavy machinery and elevated flood risks. Many Gleysols developed from C-rich holocenic sediments (Fig. 3.5). Furthermore, Gleysols may accumulate C due to oxygen limitation both processes mask potential effects of land use on TOC in subsoils. If the different TOC contents in subsoils of cropland and grassland were due to land use, the relative difference between the TOC contents of cropland and grassland should have decreased with depth. However, the opposite was the case: the relative difference was lowest in 10–30 cm, where TOC content under grassland was 1.27 times (95 % CI, 1.21 to 1.33) greater than that under cropland. Below

30 cm, the relative difference between grassland and cropland increased again to 1.62 times (95 % CI, 1.41 to 1.90) higher TOC contents under grassland than that under cropland in 70–100 cm soil depth. Overall, TOC predictions were better in 0–10 cm (R^2 of 0.70) than below this depth (R^2 from 0.39 to 0.45). Including the TOC contents of 0–10 cm as an additional predictor of TOC in > 10 cm depth improved model performance considerably, confirming that TOC contents were site-specific and that TOC in topsoil and subsoil was related (Fig. B.6). The importance of TOC in 0–10 cm for explaining TOC below 10 cm depth decreased with greater depth.

Depth gradients of TOC, which were expressed as normalised TOC values, depended less on clay content than was the case with TOC values of bulk soil (Fig. 3.2). Instead, normalised TOC values were related more to land use and soil horizons. In the upper 30 cm of grassland, TOC content decreased much more with depth than it did under cropland (Fig. 3.1), which is why the effect of land use on normalised TOC was most pronounced in 10–30 cm depth (Fig. 3.2). In 30–70 cm, differences between soil horizons were most important for explaining normalised TOC values. For example, in 30–50 cm, M horizons and A horizons still contained 43 % of TOC in 0–10 cm (95 % CI, 42 to 45), while the other master horizons contained only 27 % of TOC in 0–10 cm (95 % CI, 26 to 27). Below 50 cm depth, geological chronostratigraphy became increasingly important for explaining normalised TOC contents, while parameters related to soil formation processes (soil horizon and soil reference group) became less important – a pattern similar to that observed for TOC values of bulk soil.

3.3.2 C:N ratio

In 0–10 cm, the mean C:N ratio of bulk soil was 11.2 (95 % CI, 11.1 to 11.3) and its interquartile range was from 9.9 to 11.7. This variation was mostly related to texture. The C:N ratio increased with increasing sand content, especially above 70 % sand, while it decreased exponentially with increasing clay content to around 10 for clay contents above 10 % (Fig. B.5). High C:N ratios clustered in particular in the “Old Drift” region (Fig. 3.3c, Fig. B.4) and the “Weser-Ems-Geest” pedo-climatic zone (Fig. 3.3d, Fig. B.4). These regions are located in north-west Germany and are characterised by historic heathland and peatland cover.

At greater depths, Random Forest identified similar drivers and performed equally well in explaining C:N ratios of bulk soil as for 0–10 cm soil depth (see above).

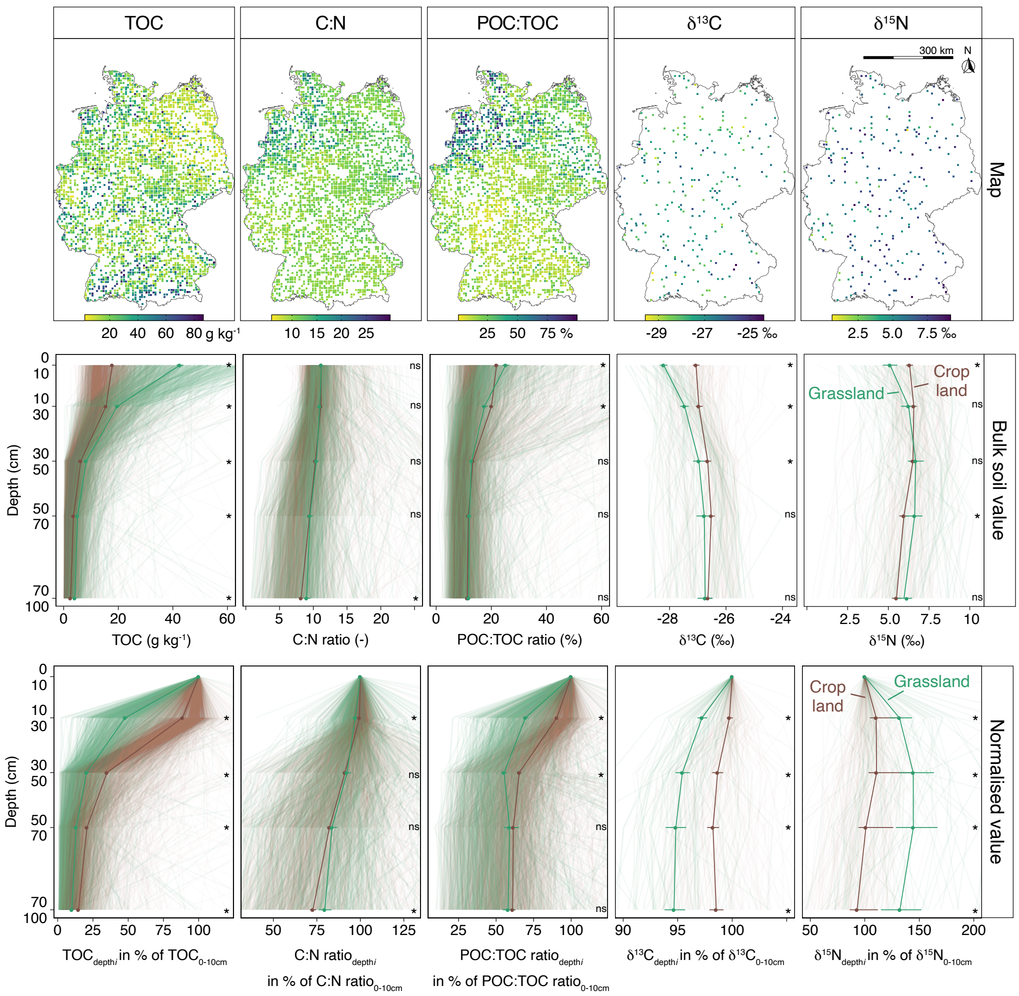


Figure 3.1: Distribution of total organic carbon (TOC) content, C:N ratio, particulate organic carbon (POC) to TOC ratio, as well as δ^{13}C and δ^{15}N values in German agricultural soils. Top row: map of bulk soil values in 0–10 cm. Middle row: depth distribution of individual and mean bulk soil values coloured by land use. Bottom row: depth distribution of individual and mean normalised values coloured by land use. Normalised values were used to describe depth gradients. Error bars illustrate bootstrapped 95 % confidence intervals around means and stars denote significant differences between means.

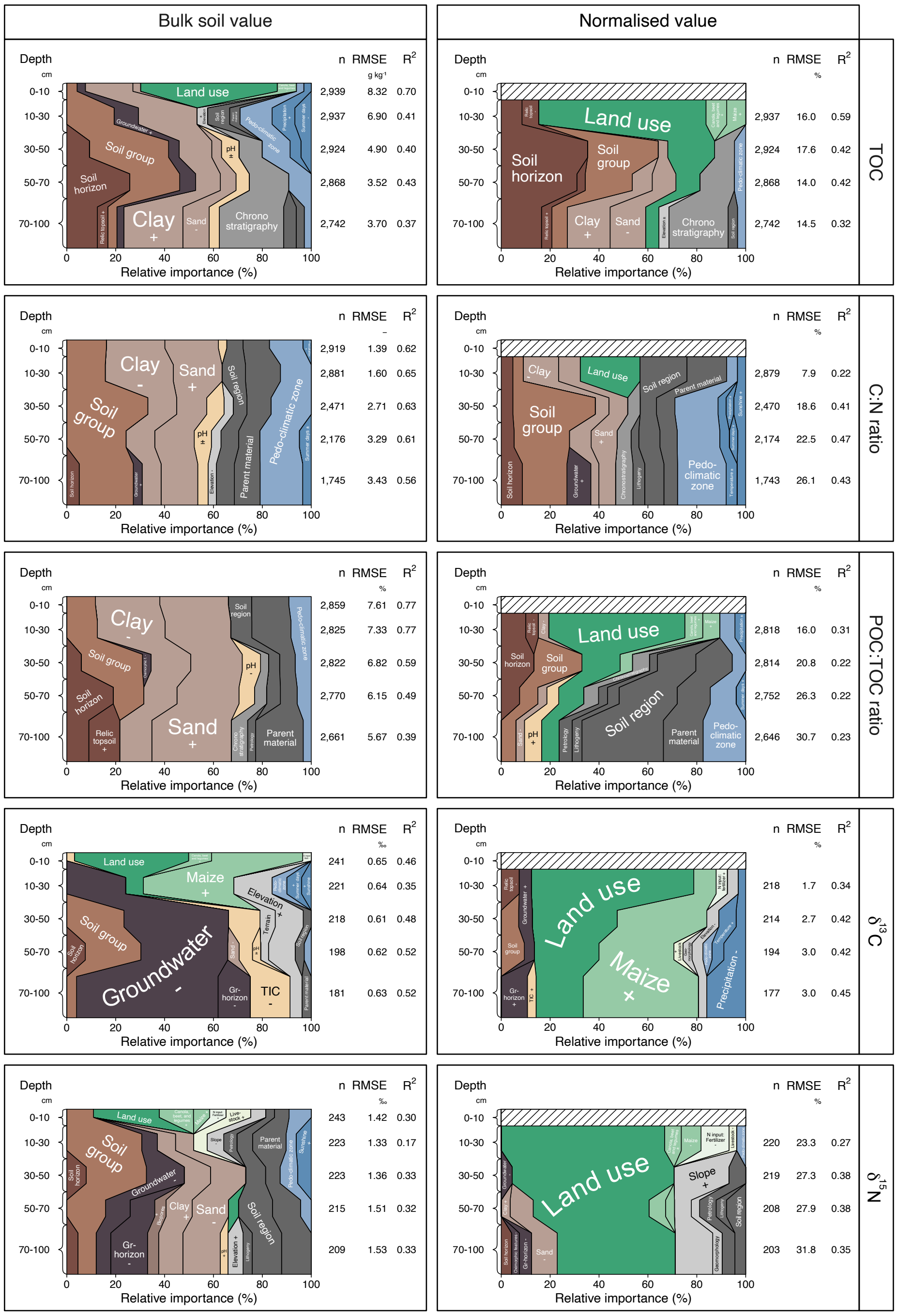


Figure 3.2: Important predictors of TOC content, C:N ratio, POC:TOC ratio, and $\delta^{13}C$ and $\delta^{15}N$ values by depth. Left: results for predicting bulk soil values without information from other depth increments. Right: results for predicting normalised values that describe depth gradients. Earthy colours represent pedology, grey represents geology and geomorphology, green represents anthropogenic influence and blue represents climate-related variables. Areas are proportional to the relative importance of variables for predicting a given target at a given depth increment. Each model is characterised by the number of observations in the training data ("n") and average errors from three times-repeated, five-fold cross validation (root mean square error "RMSE" and R-squared "R^2").

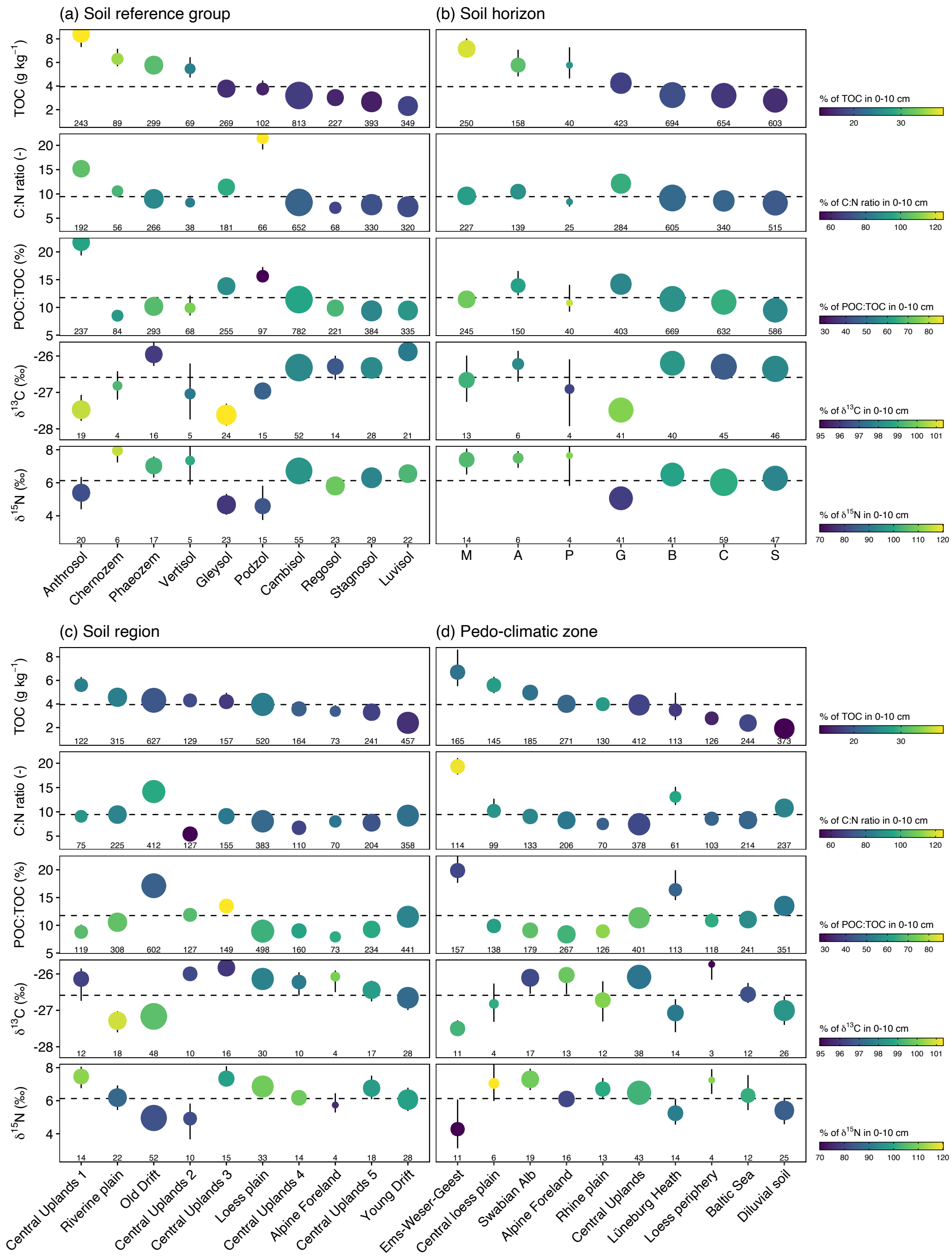


Figure 3.3: TOC content, C:N and POC:TOC ratios, and $\delta^{13}C$ and $\delta^{15}N$ values in 50–70 cm depth by (a) WRB soil reference group, (b) soil horizon ("Horizonthauptsymbol"), (c) soil region ("Bodenregion"), and (d) pedo-climatic zone ("Bodenklimaraum"). Colours illustrate normalised values, which describe depth gradients. Size illustrates sample numbers. Dashed horizontal lines represent global mean values. For better clarity, only the most important factor levels are shown (for variables with more than ten factor levels, this is the ten most common levels; only factor levels with more than three observations in $\delta^{13}C$).

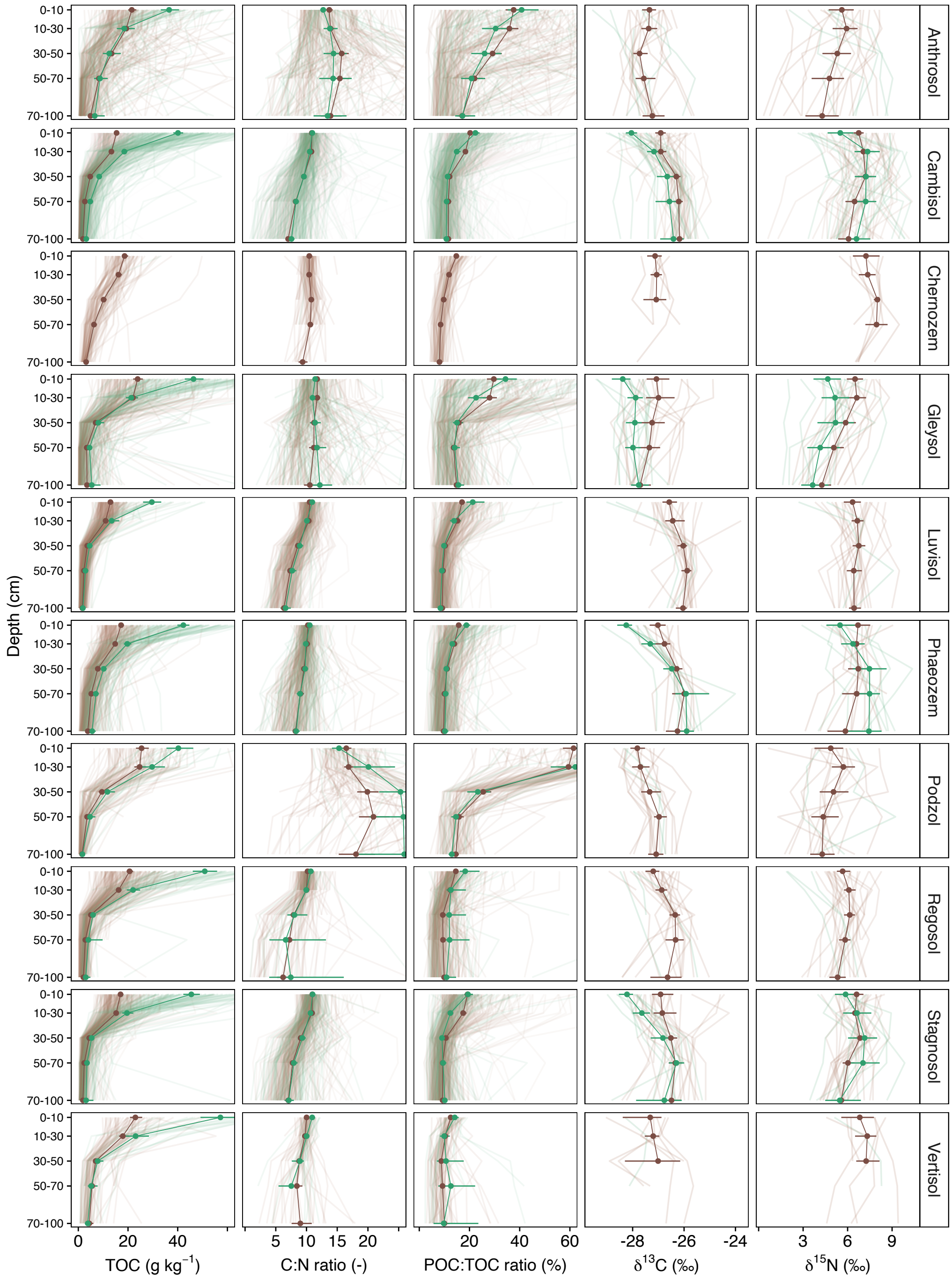


Figure 3.4: Individual and mean depth distributions of TOC content, C:N and POC:TOC ratios, and δ^{13}C and δ^{15}N values for cropland (brown) and grassland (green) by WRB soil reference group. Means are only shown for $n > 5$. Error bars illustrate bootstrapped 95 % confidence intervals of the means.

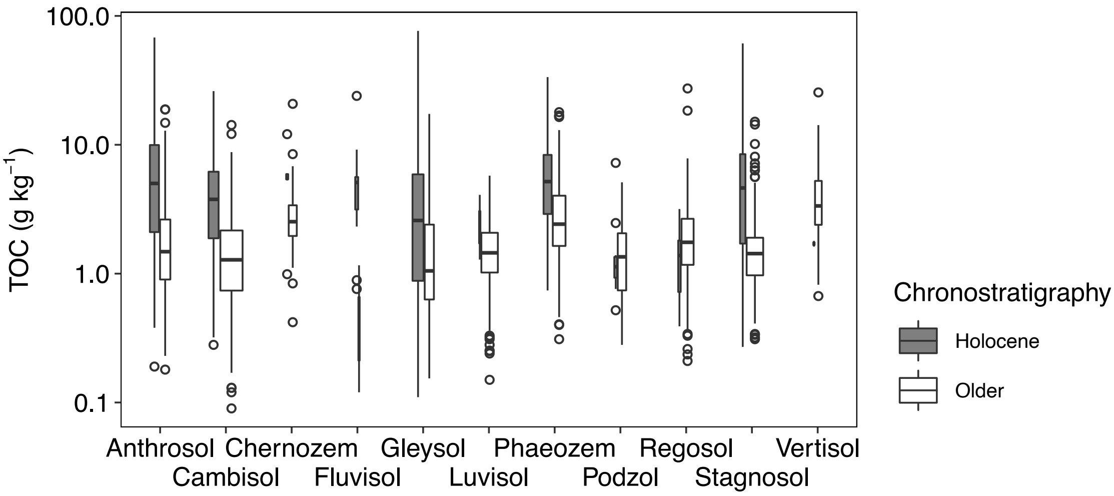


Figure 3.5: Total organic carbon content in 70–100 cm depth by soil group and chronostratigraphy. Box-plot width illustrates observation numbers.

In 30–70 cm, differences in C:N ratios by soil reference groups were most pronounced (Fig. 3.3a, Fig. 3.4) and consequently the variable importance of soil reference groups increased (Fig. 3.2). This was particularly because Podzol soils showed remarkably wide C:N ratios in subsoils. The C:N ratio of Podzols increased with greater depth, which was different to all the other soil reference groups (Fig. 3.3a, Fig. 3.4). Surprisingly, at all depth increments, the C:N ratio of cropland and grassland was very similar (Fig. 3.1) and consequently land use was not acknowledged as being important for predicting C:N ratios (Fig. 3.2). The site-specific nature of C:N was highlighted by a strong improvement of models for subsoil C:N when informed about the respective C:N ratio in 0–10 cm (Fig. B.6). The C:N ratios changed much less with increasing soil depth than TOC. In 70–100 cm depth, bulk soil C:N still constituted 75 % of bulk soil C:N ratios in 0–10 cm (95 % CI, 73 to 76). Even land use and tillage introduced only minor changes in the depth distribution of C:N ratios (Fig. 3.1). Normalisation of C:N ratios, i.e., expressing C:N ratios in terms of the percentage of their values in 0–10 cm, made land use important as a predictor of the ratios in 10–30 cm. It also increased the importance of groundwater and geological chronostratigraphy, whereas soil texture had less explanatory power (Fig. 3.2, Fig. B.4).

3.3.3 POC:TOC ratio

The POC:TOC ratio showed the most distinct regional pattern of all the organic C indicators examined in this study (Fig. 3.1). In north-west German lowlands, bulk soil POC:TOC ratios above 30 % were widespread in 0–10 cm of soil, while other regions had lower POC:TOC ratios. As for C:N ratios, soil texture and variables identifying historic heathland and peatland cover were most important for predicting POC:TOC ratios in 0–10 cm soil depth (see “Old Drift” in Fig. 3.3c; “Weser-Ems-Geest” in Fig. 3.3d). The POC:TOC ratio decreased exponentially with increasing clay content (Fig. B.5).

With increasing depth, mean POC:TOC ratios decreased from 20 % (95 % CI, 19 to 20) in 0–10 cm to 11 % (95 % CI, 11 to 12) in 70–100 cm depth. Despite this decrease, the importance of explanatory variables hardly changed with depth, and texture remained the most important explanatory variable, which made POC:TOC in 0–10 cm a good predictor of POC:TOC at greater depths (Fig. B.6). Major variations in subsoil POC:TOC were mostly associated with human soil profile modifications (Anthrosols, Fig. 3.4) and topsoil burial. Normalised POC:TOC ratios, which show the differences between sampling depths, were largely independent of soil texture, in contrast to the POC:TOC ratios of bulk soil. Instead, normalised POC:TOC ratios were driven by land use, soil reference group, soil region, parent material and pedo-climatic zone. In cropland, POC:TOC ratios decreased more gently with increasing depth than in grassland (Fig. 3.1). Podzols showed a much stronger decline of POC:TOC ratios with depth than other soil reference groups, even though the C:N ratio in Podzols increased with depth (Fig. 3.3a, Fig. 3.4). In the “Old Drift” soil region and “Ems-Weser-Gest” pedo-climatic zone, which both had historic heathland and peatland cover, POC:TOC ratios declined much more strongly along the soil profile than in other regions (Fig. B.4).

3.3.4 δ^{13}C

In 0–10 cm, the mean δ^{13}C value was −27.4 ‰ (95 % CI, −27.5 to −27.2), and differences in soil δ^{13}C were mostly explained by land use and the proportion of maize in the crop rotations (Fig. 3.2, Fig. 3.6). The mean δ^{13}C value in the upper 10 cm of grassland was −28.2 ‰ (95 % CI, −28.3 to −28.1) and that of cropland without maize was at −27.4 ‰ (95 % CI, −27.5 to −27.2).

The mean δ^{13}C value increased along the soil profile, reaching −26.7 ‰ (95 % CI, −26.8 to −26.5) in 70–100 cm (Fig. 3.1). Below 30 cm depth, groundwater ex-

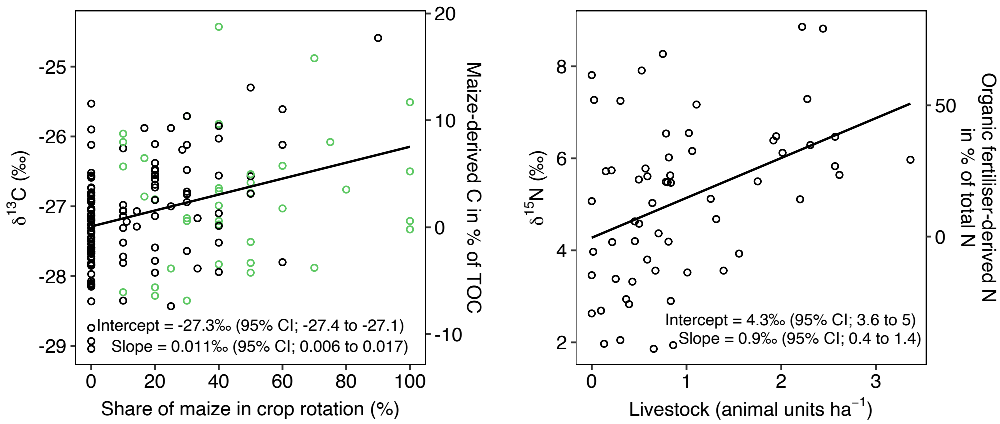


Figure 3.6: Natural abundance of ^{13}C and ^{15}N in the upper 10 cm of bulk soil. Left: δ^{13}C in cropland as a function of maize in crop rotations. Green colour shows sites where maize was the last crop before sampling. The secondary y-axis shows the proportion of maize-derived carbon (C) assuming a two-pool mixing model with the mean δ^{13}C without maize (-27.3 ‰) for the C_3 source and -12 ‰ for the C_4 source. Maize was the only C_4 crop included in the crop rotations. Right: δ^{15}N in grassland as a function of livestock units per hectare. The secondary y-axis shows the share of organic fertiliser-derived nitrogen (N) assuming a two-pool mixing model with the mean δ^{15}N without livestock (4.3 ‰) for plant litter-derived N and 10 ‰ for organic fertiliser.

plained most of the variation in δ^{13}C (Fig. 3.2, Fig. 3.7). δ^{13}C correlated negatively with the groundwater table. In 70–100 cm, soil with mean groundwater tables shallower than 80 cm showed a mean δ^{13}C value of -27.7 ‰ (95 % CI, -28.0 to -27.5), while soil with groundwater tables deeper than 200 cm showed a mean δ^{13}C of -26.3 ‰ (95 % CI, -26.4 to -26.1). Similarly, in horizons with groundwater causing reducing conditions (Gr-horizons), an average δ^{13}C value of -27.7 ‰ (95 % CI, -28.0 to -27.5) was detected, while in other horizons δ^{13}C was -26.5 ‰ (95 % CI, -26.6 to -26.4) in 70–100 cm depth (Fig. 3.7). Furthermore, in 70–100 cm, δ^{13}C of TOC decreased with increasing TIC content. Subsoil δ^{13}C values below 50 cm depth were independent of the δ^{13}C in the surface soil (0–10 cm) due to the dominant influence of groundwater (Fig. B.6). Cropland use and maize crops in particular smoothed the depth gradient of δ^{13}C since maize as a C_4 plant enriched ^{13}C in the topsoil (Fig. 3.7). Generally, changes in δ^{13}C along the depth profile were relatively small, with Gr-horizons in 70–100 cm even containing slightly more ^{13}C than in 0–10 cm depth (mean 101 %;95 % CI, 99 to 103).

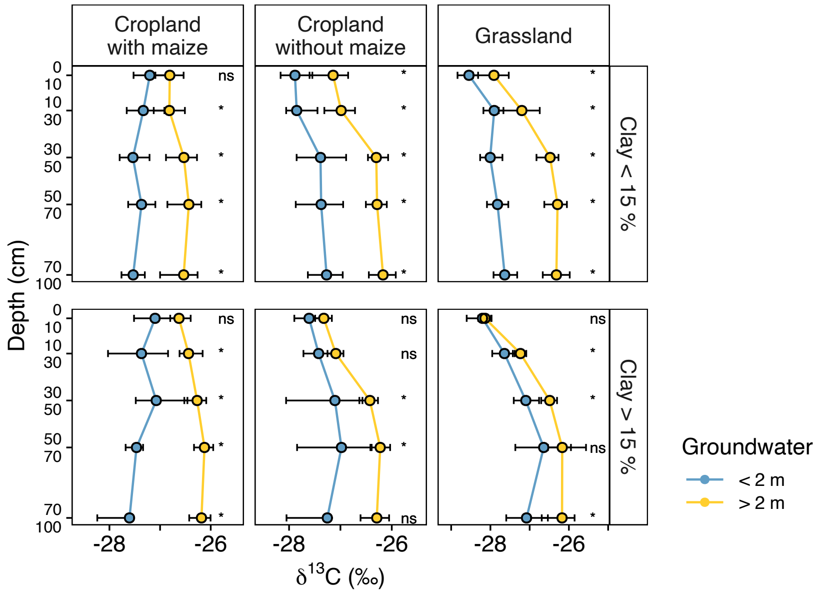


Figure 3.7: Mean δ^{13}C values of bulk soil by land use, soil texture and groundwater level. Error bars represent bootstrapped 95 % confidence intervals and stars denote significant differences.

3.3.5 δ^{15}N

In 0–10 cm, the mean δ^{15}N value was 6.0 ‰ (95 % CI, 5.8 to 6.2). With increasing depth, δ^{15}N increased to 6.6 ‰ (95 % CI, 6.3 to 6.8) in 30–50 cm before it decreased again and reached 5.6 ‰ (95 % CI, 5.4 to 5.9) in 70–100 cm (Fig. 3.1). In 0–10 cm, differences in bulk soil δ^{15}N were mostly due to land use, management and variables identifying historic heathland and peatland in north-west lowlands (Fig. 3.2). In 0–10 cm depth, the δ^{15}N value under cropland was 1.2 ‰ points (95 % CI, 0.7 to 1.7) higher than under grassland. Generally, δ^{15}N correlated positively with the proportion of canola (Brassica napus), beet (mostly Beta vulgaris) and legumes (mostly Trifolium sp.) in crop rotations (Fig. 3.2). Additionally, soil δ^{15}N values under both cropland and grassland were significantly lower in the "Ems-Weser-Geest" and "Old Drift" regions than in other regions (Fig. 3.3c, d). In grassland topsoil, soil δ^{15}N was positively correlated with livestock density (Fig. 3.6). In the subsoil, land use and management lost explanatory power; instead, soil reference group and groundwater were important for predicting δ^{15}N. In 70–100 cm depth, Gr-horizons were depleted in ^{15}N, showing 2.4 ‰ (95 % CI, 1.9 to 2.8) lower δ^{15}N values than other horizons. At this depth, δ^{15}N in Gr-horizons averaged 78 % of δ^{15}N in 0–10 cm (95 % CI, 66 to 110), while in other horizons δ^{15}N averaged 104 %

of $\delta^{15}N$ in 0–10 cm (95 % CI, 98 to 112). The depth gradient of $\delta^{15}N$ was thus best described by land use and groundwater influence. $\delta^{15}N$ values under grassland increased more with greater depth than they did under cropland because of lower values in the surface soil (Fig. 3.1).

3.3.6 Turnover of maize-derived soil carbon

Every growing season with maize increased the $\delta^{13}C$ value of cropland soil by on average 0.11 ‰ points (95 % CI, 0.06 to 0.17) in 0–10 cm depth (Fig. 3.6). Based on Eq. 3.1, this translates to a mean turnover rate of 0.7 %TOC year^{-1} (95 % CI, 0.4 to 1.1). In 10–30 cm depth, the C turnover rate was very similar (mean 0.7 % TOC year^{-1}; 95 % CI, 0.3 to 1.1). These turnover rates indicate that C resides in the ploughing layer for around 100 to 300 years on average before being released back again into the atmosphere. Below 30 cm depth, the proportion of maize in crop rotations did not correlate with $\delta^{13}C$, which is why turnover and residence time of subsoil C could not be determined.

3.3.7 Soil compaction vs. root-derived deep C input

In cropland soil with hardpans, TOC content and C:N ratio declined more with increasing depth than in cropland soil without hardpans (Fig. 3.8). Their normalised values, i.e., values at depth$_i$ relative to values in 0–10 cm, decreased significantly at increasing levels of soil compaction. The magnitude of this effect decreased with increasing soil depth. The above pattern was similar for POC:TOC ratios, but the significance here was not consistent between depth increments. In contrast to our initial hypothesis, the depth gradients of $\delta^{13}C$ and $\delta^{15}N$ values seemed not to be influenced by hardpans and showed no consistent trends with soil compaction.

3.4 Discussion

The current study is the first to provide a representative picture of the depth gradients of C:N, POC:TOC, $\delta^{13}C$ and $\delta^{15}N$ in Germanys mineral agricultural soils. Based on the large number of soil samples (2931 sites * average of 5.4 depth increments) and high data quality (all soil analyses in one laboratory), our data-mining approach revealed previously unseen patterns in TOC depth distribution and soil organic matter quality to 100 cm depth at regional scale. In the following,

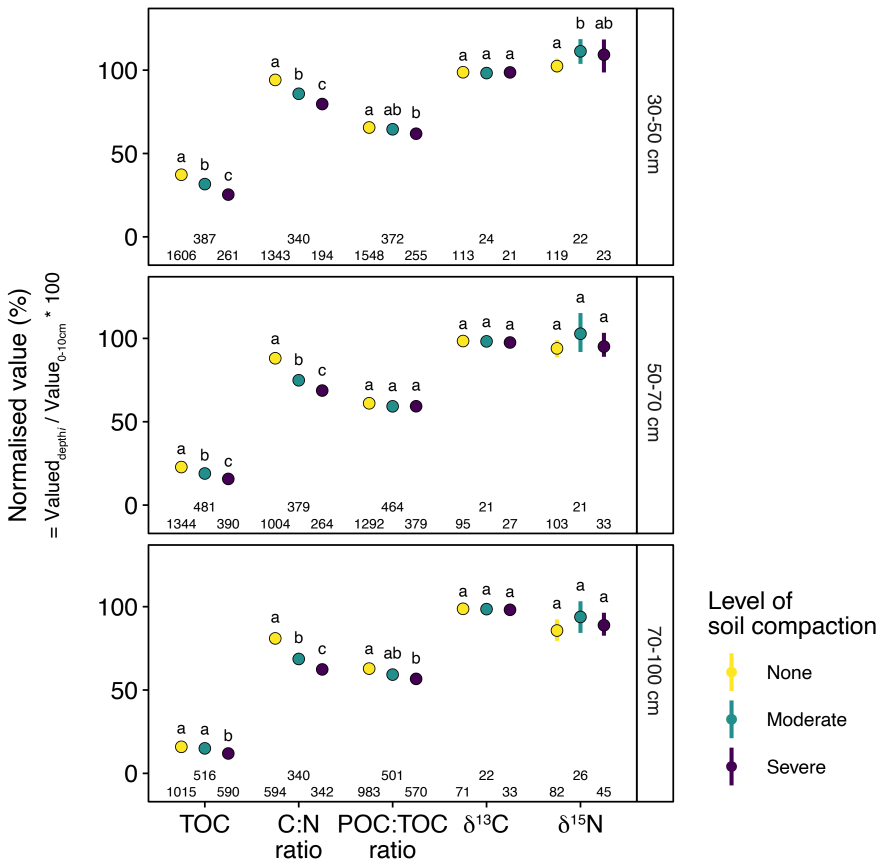


Figure 3.8: Normalised TOC, C:N, POC:TOC, δ^{13}C and δ^{15}N values in cropland soil without compaction, moderate compaction and severe compaction. Mean values are shown with error bars representing bootstrapped 95 % confidence intervals. Different letters indicate significant differences at the 5 % level.

we discuss how these patterns can be used to trace different entry paths of organic C into German agricultural soils. We differentiate between:

- autochthonous C, which covers aboveground and belowground C inputs from plants that grew on top of a given soil profile
- C input from organic fertiliser (animal excreta), and
- parent material-inherent C, which comprises allochthonous C from plants that once grew somewhere else, e.g., upslope or upstream.

Also, we discuss the importance of vertical redistribution within soil profiles for explaining subsoil C, as well as texture and groundwater as major causes of variable C retention in German agricultural soils.

3.4.1 Origin of topsoil carbon

Most organic C entered the topsoil in the usual way, i.e., it originated from plants that grew on top of a given agricultural land, and not from somewhere else, and is therefore of autochthonous origin. The natural label of maize-derived C allows these autochthonous C inputs to be quantified. Our results suggest that each cropping year with maize replaced 0.3 % to 1.1 % of TOC in the upper 30 cm of cropland. Poeplau et al. (subm) estimate German cropland to store on average 61 Mg TOC ha^{-1} in 0–30 cm (mineral soils only). Thus, autochthonous C contributed to the current soil organic C stock of German cropland at a mean rate of 0.2 to 0.7 Mg C ha^{-1} $year^{-1}$. This estimate is about one order of magnitude lower than the C input of 3.2 Mg C ha^{-1} $year^{-1}$, which was recently proposed by Jacobs et al. (subm). However, the number of Jacobs et al. (subm) refers to all plant residues and photosynthates that are not harvested, including stubble, mulch and other litter material $>$ 2 mm. Soil organic C, however, includes only the organic C moieties $<$ 2 mm. Plant residues $>$ 2 mm have to be decomposed before entering the soil organic C pool. Decomposition is accompanied by respiration and organic C losses, which explains why less than 25 % of the initial 3.2 Mg C input ha^{-1} $year^{-1}$ that remains in the fields after harvest finally ends up in the fine soil. Once in the fine soil, organic C is likely to remain there for a mean period of 100 to 300 years before being mineralised and released back into the atmosphere. This mean residence time represents a rough approximation assuming steady state conditions and first-order decomposition rates (Gleixner et al., 2002) - we did not perform radiocarbon dating. Uncertainties also remain from the use of single-pool mixing

models; due to uncertain data in the long term we did not perform estimations using two-pool C concepts (Derrien & Amelung, 2011). Nevertheless, our estimate is in good agreement with commonly reported radiocarbon ages of TOC in the ploughing layer (e.g., Flessa et al., 2008).
Our method of calculating organic C turnover differed from most previous studies and contains additional uncertainties. Our calculations are based on: (i) sites with crop rotations instead of continuous maize cultivation, (ii) unknown maize-derived C inputs dating back more than 10 years, and (iii) about 170 core sites instead of just one or a few sites. We believe that (iii) compensates for potential noise introduced by (i) and (ii). Once organic C has entered the fine soil, the vast majority resides there for $>>10$ years. We did not observe a systematic pattern between the time period since the last maize crop and the $\delta^{13}C$ value of soil (Fig. 3.6, green dots). Hence, the exact timing of the last maize cropping in the past 10 years barely influenced organic matter turnover estimates in the range of 100 years and beyond. Unknown historic maize-derived C input was a potential source of bias in our turnover calculation. If the recorded share of maize in crop rotations within ten years before sampling correlated with historic maize use, we would have over-estimated TOC turnover. However, this seems unlikely since our estimate for C turnover (0.3 % to 1.1 % of TOC $year^{-1}$) is at the lower range of what has previously been observed in field trials. Schiedung et al. (2017) reported much faster C turnover: here, after two years, maize-derived C had substituted 7.4 ± 3.2 % of TOC in the topsoil (0–30 cm) and 2.9 ± 1.7 % of TOC in the subsoil (30–50 cm), yet in their study shredded maize stubble was left as mulch on the soil surface, probably enhancing maize-derived C input into the topsoil. Flessa et al. (2000) reported that 15 % of TOC in 0–30 cm was maize-derived after 37 years of continuous maize cropping, which translates into a turnover of 0.4 % of TOC $year^{-1}$. Rasse et al. (2006) estimated topsoil organic C turnover to be 1.0 % of TOC $year^{-1}$ for a Eutric Cambisol site in France. We therefore conclude that the simplified estimation of our turnover rate at 0.3 % to 1.1 % of TOC $year^{-1}$ is a reasonable magnitude for TOC turnover in the ploughing layer of German cropland.
In grassland, $\delta^{15}N$ values were indicative of additional C and N inputs in the form of organic fertilisers. Elevated $\delta^{15}N$ values in the topsoil of grassland with high livestock densities indicated a significant proportion of soil N to be derived from slurry or manure. Slurry-derived and manure-derived N tends to be enriched in ^{15}N because of isotopic discrimination during digestion and ammonia volatilisation

during storage, resulting in δ^{15}N values ranging from 6 ‰ to 13 ‰ (Kriszan et al., 2014). Each unit (500 kg) increase in livestock per hectare increased δ^{15}N of grassland in 0–10 cm by on average 0.9 ‰. This slope is in perfect agreement with the one documented by Kriszan et al. (2014), who studied the effect of stocking rates on δ^{15}N in the upper 5 cm of nine grassland sites in western Germany. Based on a positive correlation between δ^{15}N in topsoil and overall farm N balances, Kriszan et al. (2014) proposed using δ^{15}N as an indicator for N-use efficiencies at farm scale. Grassland of farms with positive N balances, i.e., greater N input than N export, showed topsoil δ^{15}N values above 5.4 ‰ (Kriszan et al., 2014). In the present study, half of all grassland sites were above this threshold value, indicating that about half of Germany's grassland shares a decadal history of N surpluses due to excessive organic fertilisation. Assuming that δ^{15}N in grassland topsoil without slurry and manure fertilisation was 4.3 ‰ (intercept of linear regression line of δ^{15}N vs. livestock), average δ^{15}N of organic fertiliser was 10 ‰ and there was similar fractionation of soil N and amended slurry/manure N, then each livestock unit increased the share of organic fertiliser-derived N under grassland and 0–10 cm by 15 percentage points (95 % CI, 8 to 22; Fig. 3.6). Considering that organic C and total N were highly correlated (grassland, 0–10 cm: $R^2 = 0.86$), the proportion of organic fertiliser-derived topsoil C can be assumed to be similar to the organic fertiliser-derived proportion of topsoil N. This estimate should be considered as a very approximate figure because divergence in both δ^{15}N of N input and fractionation factors for δ^{15}N in soil can be huge (Craine et al., 2015; Högberg, 1997) – much higher than for δ^{13}C. Nonetheless, the effect of livestock on δ^{15}N values in soil indicates that in addition to plant-derived C input, manure-derived and slurry-derived C has also contributed significantly to topsoil C stocks in German grassland.

The Random Forest algorithm identified systematic patterns in TOC contents, C:N and POC:TOC ratios between sampling sites and depths. These patterns were indicative of land use and management-driven differences in the quantity and quality of C inputs and subsequent redistribution of these inputs. In 0–10 cm, land use was the most important predictor of TOC and grassland showed a TOC content 2.4 times greater than cropland. This might be explained by grassland typically receiving a greater total root-derived C input than cropland (Don et al., 2009). Root-derived C resides in soil longer than other types of C input (Rasse et al., 2005). This supports the hypothesis that higher TOC content in grassland compared with that in cropland is caused by different quantities of root-derived

C input. Differences in TOC contents by land use were further amplified by tillage-induced redistribution of TOC under cropland. Most cropland in Germany is ploughed annually to an average depth of about 30 cm, which decreases TOC content in 0–10 cm and increases it in 10–30 cm. Thus, differences in the depth gradient of TOC in the upper 30 cm between grassland and cropland arose from both different C input and tillage-induced redistribution. Both processes together explain the large land use effects on the depth gradients of TOC contents, as well as of POC:TOC and $\delta^{13}C$ and $\delta^{15}N$ values (Fig. 3.2, right) tillage effects could not be separated from C input effects.

Interestingly, in 0–10 cm, Random Forest considered land use to be the most important variable for explaining TOC, but irrelevant for explaining absolute C:N and POC:TOC ratios (Fig. 3.2, left). This was surprising considering the greater root-derived C input and much less frequent or absent tillage in grassland compared with cropland. A higher TOC content at equal C:N and POC:TOC ratios in grassland than in cropland can only be explained if both POC and MOC were equally elevated under grassland, indicating that the amount of MOC in the topsoil is governed not only by texture but by input as well: under steady state conditions, topsoil MOC content thus also increases with increasing C input (Rehbein et al., 2015).

In addition to recent land use and management effects on topsoil TOC, our study confirmed the legacy effects of historic heathland and peatland cover on organic C quality and quantity unique to the north-west part of Germany (Vos et al., 2018). Here, the maritime climate with relatively large amounts of rain in combination with forest clearances and subsequent spread of heathland favoured the podzolisation of old drift sands (Behre, 2008; Schmidt & Roeschmann, 2014). Ironpans that developed during podzolisation hindered water drainage and favoured the spread of peatland on a large scale. In the last few centuries, most of the peatland has been drained, the peat harvested, ironpans broken and former heathland and peatland converted to agricultural land (chapter 5). Today, the affected soils still have an elevated TOC content (Springob & Kirchmann, 2002), C:N ratios > 13 (Poeplau et al., subm) and POC:TOC values > 30 % (Vos et al., 2018). Detailed information about the extent of the historic heathland and peatland is limited and therefore could not be included as a covariate in this study. However, the region in which historic heathland and peatland have been found is characterised by a distinct climate (considerable rain, limited sunshine, mild winters), soil region (Old Drift), parent material (drift sand) and the pedo-climatic zone (Weser-Ems-Geest). Therefore, these variables informed the Random Forest models about historic heathland and peatland cover. Direct climate effects on recent C inputs or C turnover could not be inferred from the present study.

3.4.2 Origin of subsoil carbon

Below 30 cm depth, the ^{13}C label of maize and the ^{15}N label of organic fertiliser could no longer be detected, which confirms at national scale what many studies have previously shown at field scale: subsoil C and N are much less responsive to management-induced differences in C and N inputs than topsoil C and N (Poeplau & Don, 2013). Subsoil C must therefore be older than topsoil C and exchanged with atmospheric C on a much longer timescale, millennial rather than centennial (Balesdent et al., 2018). In the Random Forest models, information on land use and management, which was recorded in the German Agricultural Soil Inventory for 10 years preceding sampling, was not relevant for explaining bulk soil TOC content below 30 cm depth. The only indication of significant exchange between subsoil C and the atmosphere was offered by the depth gradients of TOC, C:N and POC:TOC in soil profiles with hardpans (Fig. 3.8, Fig. B.7). Below hardpans, TOC contents as well as C:N and POC:TOC ratios were relatively low, suggesting that hardpans significantly restricted root-derived litter input into subsoils. This confirms the existence of root-derived C inputs to the subsoil. However the question remains of how much deep roots and their rhizodeposits contribute to the TOC stocks of subsoils. If organic C were solely root-derived and the input of root-derived C were only a function of depth, it should be possible to predict the organic C quantity and quality along the soil profile from the organic C quantity and quality of the topsoils. However, the importance of topsoil C in 0–10 cm for explaining subsoil C decreased with increasing depth (Fig. B.6), suggesting that:

- C input is not only a function of depth but also of root-restricting soil properties
- the contribution of translocated C or parent material-inherited C increases with increasing depth, and/or
- with increasing depth, texture-driven differences in the residence time of C increase subsoil C is governed more by clay content than by root-derived C input.

This last point of texture-driven C retention has a huge effect on TOC storage, especially in the subsoil. Deep in the soil profile, C input is typically low and C stabilisation governs how much C is being stored. Given two subsoils that only differ in C input, the subsoil receiving the higher C input will also show the larger TOC content. However, if a third subsoil not only differs in C input but also in soil texture, interpreting its TOC content is not straightforward because texture is key to C retention. This makes separating the effects of C input and C stabilisation challenging at sites with different textures. At a regional scale, however, as in German agricultural soils, texture tends to vary much more between sites than with soil depth[1], therefore texture-driven differences in C retention can be overcome by evaluating depth gradients of TOC instead of independent bulk soil values. Depth gradients allow inferences to be drawn about the depth distribution of organic C inputs even at sites with contrasting soil textures.

In the present study, we used a Random Forest algorithm to elucidate patterns behind the depth gradients of organic C in Germanys agricultural soils. To explain the depth gradients of TOC contents as well as C:N and POC:TOC ratios, the algorithm ranked variables and indicated that soil parent materials, soil transport and vertical translocation of C were most important. About 35 % of agricultural soils developed from relatively young, holocenic deposits, most of which were either of fluvio-marine or colluvic origin. Such alluvial and colluvial sediments typically comprise large amounts of allochthonous C from upslope or upstream areas (Doetterl et al., 2012) and can bury significant amounts of autochthonous C at their depositional sites (Chaopricha & Marn-Spiotta, 2014). In view of elevated subsoil C contents and only minor decreases of TOC in soil profiles from holocenic deposits (Fig. 3.5), we hypothesise a significant proportion of allochthonous C and buried autochthonous C to be still preserved in subsoils. Floodplains and wide valley bottoms are widely acknowledged to act as major C sinks in the landscape (Sutfin et al., 2016). Hoffmann et al. (2009) estimated the non-alpine part of the Rhine basin to have accumulated about 1 Pg of organic C from upstream and upslope areas since the beginning of the floodplain deposition, which translates to a mean Holocene sequestration rate of roughly 50 kg C ha^{-1} $year^{-1}$. Recent C sequestration rates in the Rhine basin are hard to quantify, but there is evidence that agricultural intensification has increased pre-human C sequestration rates of the Rhine basin by at least one order of magnitude due to stronger hillslope

[1] In German agricultural soils, the average interquartile range of clay within soil profiles was roughly three times lower than the interquartile range of clay between sites.

erosion (Hoffmann et al., 2013). This highlights the importance of lateral C fluxes in explaining soil organic C stocks, especially (i) when moving beyond pedon to landscape and regional scales (van Oost et al., 2012), and (ii) for explaining subsoil C stocks due to their lower C turnover than topsoils. Organic C inherited from holocenic, i.e., relatively young, soil parent material appears to be a key contributor to subsoil C stocks in German agricultural soils.

Another major contributor to subsoil C was topsoil C translocated into the subsoil via anthropogenic soil profile modifications (e.g., deep ploughing), bioturbation (e.g., in Chernozems) and eluviation (e.g., in Podzols). Numerous agricultural soil profiles have been modified by farmers far beyond annual tillage depths with the goal of site melioration. Such Anthrosols showed much higher TOC contents, and wider C:N and POC:TOC ratios in subsoils than most other soil groups. The depth gradients of these parameters were very noisy in Anthrosols (Fig. 3.4) but these depth gradients were also less steep on average than in other soil groups (Fig. 3.3a). The noise in the depth gradients of Anthrosols illustrates the diversity of their underlying formation. Anthrosols comprise a large variety of soils that have all been modified profoundly by human activity, including deep-ploughed soil, mining overburden, landfills and plaggen soil. Most deep soil profile modifications have accidentally translocated and buried great amounts of topsoil C in deeper soil layers. Previous studies have shown that such topsoil burial increases the residence time of C and thus soil organic C storage (Alcántara et al., 2016). Anthrosols mostly occurred either in the Old Drift landscape of north-west Germany or in viticultural areas along the Rhine and Mosel rivers, but they covered a significant proportion (8 %) of agricultural land in Germany, making anthropogenic soil profile modifications an important feature for explaining the variability in subsoil C stocks and organic C depth gradients at national scale.

Furthermore, soil biota seems to have transferred great amounts of topsoil C into the subsoil. In the German soil classification (AD-HOC-AG Boden, 2005), epipedon with strong bioturbation is coded with the soil horizon symbol “Ax”. On average, Ax-horizons reached a depth of 76 cm (95 % CI, 74 to 80). Most “Ax”-horizons occurred in Chernozems, which interestingly showed relatively high TOC but relatively low POC:TOC values in subsoils compared with other soil groups (Fig. 3.3a). This could be explained by the activity of anecic earthworms, which might not only bury topsoil C but also convert particulate organic matter to mineral-associated organic matter and thus decrease POC:TOC ratios (Vidal et al., 2019).

Finally, some topsoil C was translocated to subsoils during podzolisation. About

3.5 % of all sampled sites were Podzols. Most of them developed from pleistocenic drift sands in north-west Germany. Podzols showed much higher C:N but lower POC:TOC ratios in subsoil compared with topsoil, indicating that instead of POC, dissolved organic C species with a high C:N ratio were illuviated in the subsoil of Podzols (Sauer et al., 2007). The great importance of the "Weser-Ems-Geest" pedo-climatic region and the "Old Drift" soil region in explaining the depth gradients of C:N and POC:TOC points to considerable amounts of refractory C from historic heathland and peatland cover in soil profiles in this region. However, many agricultural soils in the "Weser-Ems-Geest" area were also subject to deep soil profile modifications (Anthrosols) or podzolisation (Podzols), which makes it difficult to disentangle the individual processes to explain elevated subsoil C in this area.

3.4.3 Effects of texture and groundwater on organic C

The close correlation between organic C content and soil texture and with variables characterising oxygen availability (depth of groundwater table, Gr-horizons) underlines their influence on the retention and turnover of soil organic matter. Clay increases the C-storage capacity of soils because it offers a large, charged specific surface area for sorption of organic C (Hassink, 1997; von Luetzow et al., 2008). Mineral-associated organic C mostly consists of organic matter with relatively low C:N ratios (Jilling et al., 2018). The observed decrease in C:N and POC:TOC ratios with increasing clay content (Fig. 3.2) can therefore be attributed to the preferential retention and microbial conversion of organic C on mineral surfaces. Sorption of organic C on clay surfaces decreases C turnover (von Luetzow et al., 2008), whereas microbes allocated on mineral surfaces directly incorporate metabolised C into their biomass and necromass (Kögel-Knabner & Amelung, 2014). This makes soil texture a key variable for explaining the C stocks of agricultural soils in Germany (Vos et al., 2019).

Groundwater can decrease C turnover because it restricts oxygen availability and therefore biological activity (Blazejewski et al., 2005; Marin-Spiotta et al., 2011). About 11 % of all examined sites show Gr-horizons, i.e., reducing conditions in at least 9 out of 12 months (AD-HOC-AG Boden, 2005). These horizons had much lower $\delta^{13}C$ and $\delta^{15}N$ values than those of other soil horizons with higher oxygen availability at similar depths. Since microbial turnover constantly enriches ^{13}C and ^{15}N in the metabolites (Boutton, 1996a), low $\delta^{13}C$ and $\delta^{15}N$ values in watersaturated Gr-horizons may indicate retarded biological decomposition (Natelhoffer & Fry, 1988).

In soil with a similar C input, different $\delta^{13}C$ values of bulk soil tended to be associated with different POC:TOC ratios. In Gr-horizons, however, $\delta^{13}C$ and also $\delta^{15}N$ were low, while POC:TOC ratios were average. Instead of retarded conversion of POC to MOC and associated changes in POC:TOC, it could be retarded MOC turnover that keeps $\delta^{13}C$ and $\delta^{15}N$ values in Gr-horizons relatively low in other horizons, MOC turnover could lead to an enrichment of heavy isotopes, particularly on the timescale of pedogenesis. Alternatively, the low $\delta^{13}C$ and $\delta^{15}N$ values observed in hydric soil could be explained by compound-specific organic matter turnover (Gurwick et al., 2008). Under anaerobic conditions, ^{13}C-enriched carbohydrates might be decomposed at a higher rate, resulting in the selective preservation of ^{13}C-depleted lignin compounds (Benner et al., 1987; Spiker & Hatcher, 1987). Finally, it should be borne in mind that some Gleysols developed from C-rich holocenic sediments. The degree to which allochthonous C from aquatic sources, which also has light isotope signatures (Finlay & Kendall, 2007; Laskov et al., 2002), contributes to the TOC content and thus to $\delta^{13}C$ and $\delta^{15}N$ values in the Gr-horizons warrants further clarification.

It is noteworthy that groundwater had a much stronger effect on bulk soil values of $\delta^{13}C$ than on its depth gradient. This was because groundwater-affected soil showed slightly more negative $\delta^{13}C$ values than sites without groundwater influence, even in topsoil. Generally, groundwater tables were too low to affect C decomposition even in the topsoil. Instead, different source signals probably contributed to the observed differences in the $\delta^{13}C$ values of topsoils. Plants growing at sites without groundwater influence might experience more frequent and severe drought stress than plants growing at sites with high groundwater levels. Under water stress, C_3 plants tend to get enriched in ^{13}C by up to 1 ‰ as a result of a decreased stomatal aperture (Boutton, 1996a). Thus, water stress-induced ^{13}C enrichment of C_3 photosynthates might explain the observed differences in $\delta^{13}C$ values of topsoils (Fig. 3.7). Together, the two processes of decreased decomposition of subsoil C at sites with high groundwater and ^{13}C-enriched-C input, especially in the topsoil at sites without groundwater influence, might explain why groundwater affected $\delta^{13}C$ values in both subsoil and topsoil in the same direction.

3.4.4 Loosening hardpans is climate smart

A significant bend in the depth gradients of TOC contents, C:N and POC:TOC ratios associated with hardpans suggests restricted deep root-derived C inputs in and below hardpans. In the case of TOC, the same trend was found even after mass correction to account for site-specific rock contents and bulk densities by evaluating depth gradients of TOC density, i.e., kg TOC ha^{-1} at $depth_i$ relative to 0–10 cm (Fig. B.7). These results confirm that loosening compacted soil layers has the potential for additional C storage in subsoils because loosening of compacted soil can facilitate deep root-derived C inputs. If loosening of compacted soils could achieve the same depth gradients of TOC density as that observed in non-compacted soil profiles, this could increase C stocks in 30–100 cm by 2.3 Mg C ha^{-1} on average. However, the site-specific C-sequestration potential of soil loosening depends on the magnitude and depth of compacted soil layers. At sites with severely compacted soil layers starting already at 30 cm depth, loosening of soils could potentially accumulate up to 9 Mg ha^{-1} additional organic C in 30–100 cm, while at sites with medium compaction only at 70–100 cm depth, loosing could increase subsoil organic C stocks by about 1 Mg ha^{-1} only. If all compacted soil layers in 30–100 cm depth were loosened so that the depth gradients of TOC density resembled those of non-compacted soil profiles, German cropland could store 0.03 Pg (4 %) more organic C in total in 30–100 cm depth. This corresponds to 119 874 thousand tonnes of carbon dioxide equivalents or 1.8 times the annual greenhouse-gas emissions of Germanys entire agricultural sector (UBA, 2019a). Considering that clay content increased with increasing level of compactness and that clay correlated slightly positively with the depth gradient of TOC, the CO_2 sequestration potential of cropland could even be greater. However, from what is known about topsoils (Poeplau et al., 2011), it is likely that subsoil C stocks would need at least a few decades to reach their new C equilibrium after soil loosening. Furthermore, deep soil loosening is not a trivial measure and might have to be repeated after a few years (chapter 5). It is generally easier to loosen shallow hardpans than those at greater depths. Loosening shallow hardpans also has greater potential for C sequestration and is thus highly promising for climate mitigation.

3.5 Conclusions

Fresh photosynthates feed the organic C stock of German cropland in 0–30 cm depth at a mean rate of 0.2 to 0.7 Mg C ha^{-1} $year^{-1}$. Organic fertiliser is another important source of C input, especially in grassland. In parts of north-west Germany, sandy soils still contain elevated amounts of historic C from past heathland and peatland cover.

In subsoils, holocenic parent material harbours large amounts of allochthonous C from upstream or upslope areas. This parent material-inherited C is a major contributor to subsoil C, especially in soils that developed from alluvial or colluvial deposits. Furthermore, vertical displacement of topsoil C along the soil profile contributed significantly to subsoil C storage in German agricultural land, especially in Anthrosols (topsoil burial), Chernozems (bioturbation) and Podzols (illuviation). Overall, the origin of parent material and related pedogenesis were key drivers of subsoil TOC storage. The only evidence of direct root-derived C input into subsoils was a significant bend in the depth profile of TOC contents as well as C:N and POC:TOC ratios in compacted soil layers, suggesting that hardpans restrict root-derived C inputs into subsoils. The sustained loosening of hardpans could increase deep root-derived C inputs and thus result in a significant increase in subsoil C stocks.

Chapter 4

Adaption and melioration

Adapted from
Schneider, F. & Don, A. (2019). Root-restricting layers in German agricultural soils. Part II: Adaptation and melioration strategies. Plant and Soil, 442(1):419-32.

4.1 Introduction

Root-restricting layers (RRLs) in agricultural soils can severely limit the plant availability of water and nutrients from subsoils. Restricted access to these subsoil resources can cause severe yield losses, especially in growing seasons with droughts (Kirkegaard et al., 2007). In Germany, the area extent of RRLs is estimated to be 71 % of total agricultural land (chapter 2). Root restrictions were mainly of physical origin (soil strength, rock fragments, bedrock), but also physico-chemically derived (acidity, anoxia). Affected farmers may either accept and adapt to RRLs or aim to improve adverse growing conditions through soil melioration (Fig. 4.1). Adaptation to RRLs may manifest itself in land use or the choice of crop type. Adjusting land use to site conditions is common practice: fertile soil with high yield potential tends to be used intensively, e.g., as conventional cropland. RRLs have been shown to decrease the fertility and potentially attainable yield of agricultural land, thus agricultural land with RRLs might preferentially be used more extensively, e.g., as grassland. If sites with RRLs continue to be used as cropland, farmers might adjust crop rotations accordingly. Crop species have different requirements for soils. For example, winter wheat grows best in medium to heavy textured soil at pH 7, while winter rye performs well on light textured soil and pH 5 to 6 (Goldhofer et al., 2014b). Thus if potential root

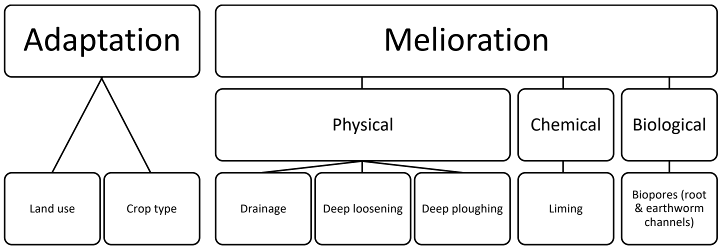


Figure 4.1: Management strategies for cultivating land with root-restricting soil layers.

restriction is caused by sandy subsoil texture or acidity, rye might be preferred over wheat.

Apart from adaptation, there are various melioration strategies for sites with RRLs. The choice of an appropriate meliorating option depends on the cause of root restriction. Anoxia is mostly caused by stagnant water or groundwater. Waterlogged soils can be drained by means of pipe or ditch systems. Successful drainage will improve the growing conditions and workability of affected sites. Root restrictions due to acidity can be overcome by liming. To meliorate acid subsoils with minimal disturbance, surface applications of gypsum have been found to be more effective than lime (Sumner, 1995). This is because of the higher mobility of gypsum compared to lime. Leaching gypsum has been found to effectively supply calcium and decrease aluminium toxicity in acid subsoils (Shainberg et al., 1989). Compacted soil can be meliorated either biologically or physically. The biological method aims to promote the formation of earthworm and root channels penetrating compacted soil (Cresswell & Kirkegaard, 1995). Subsequent crops could then use these biopores as highways into deeper soil layers (Kautz, 2015). Taprooted cover crops can increase biopore density in soils (Han et al., 2015a). The thicker the root, the greater its ability to elongate in compacted soil (Materechera et al., 1992). Most dicotyledonous plants form thicker roots than monocotyledons (Klepper, 1992), therefore dicotyledons such as alfalfa have been suggested for meliorating compacted soil (Kautz, 2015; Lynch & Wojciechowski, 2015). A successful biological melioration of compacted soil is often cheaper and more persistent than physical melioration options (Shaxson & Barber, 2003). The main disadvantage of meliorating compacted soil biologically is the time this management option requires: recuperation takes one to three years, during which the affected land has to be taken out of production. Physical melioration of compacted soil is much faster. Deep chiselling (= subsoiling or deep ripping) can loosen compacted soil layers mechanically down to 1 m depth (chapter 5). However, mechanically loosened soil is susceptible to re-compaction. This re-compaction can be slowed down by decreasing trafficking intensity, particularly while soil is wet. The latter has often been neglected in the past, which may explain why many practitioners consider mechanical deep loosening effects as short-lived while controlled field experiments, which avoided traffic and promoted biological stabilisation show that mechanical loosening can indeed be long-lived (chapter 5). Traffic-induced re-compaction of loosened soil might be slowed down by incorporating compost and other organic matter-rich substrate into the subsoil (Frelih-Larsen et al., 2018; Jakobs et al., 2017). However, this management option is still in its test phase. Apart from mere soil loosening, soil profiles can also be ploughed, flipped or mixed up to 2 m depth to meliorate compacted subsoil layers. Such management options typically require large amounts of organic fertiliser and lime to replenish topsoil fertility after melioration (Bechtle, 1985). This explains why ploughing, flipping or mixing of soil profiles are performed only rarely to overcome soil compactness. However, in New Zealand, soil flipping is successfully applied on large scales to remove ortsteinic hardpans in subsoils and improve water infiltration of soils under grassland use (Schiedung et al., 2019). Furthermore, in northwest Germany large regions were drained and deep ploughed several decades ago to convert former peatland and heathland into agricultural land (Alcántara et al., 2016).

Numerous strategies for managing sites with RRLs are in place and used differently depending on soil, environmental and socioeconomic conditions. However, there is no comprehensive overview of melioration measures that are applied in practice. In this study, the first German Agricultural Soil Inventory (Jacobs et al., 2018) was used to assess the popularity of common strategies for subsoil management in Germany. Specifically, the aims of this study were (i) to compare land use and characteristic crop types on sites with and without RRLs, (ii) to estimate the area extent of agricultural land with physicochemical melioration (deep tillage, drainage or liming), (iii) to examine the likelihood of physicochemical melioration based on pedologic, geologic, climatic and socioeconomic characteristics, and (iv) to identify pedogenic constraints to meliorating compacted subsoil layers by earthworm and root channels.

4.2 Materials & Methods

4.2.1 The dataset

The dataset of the first German Agricultural Soil Inventory (2011–2018) contains information on soil, geology, land use and management of 3078 sites covering German agricultural land in a 8 km x 8 km grid (Jacobs et al., 2018). At each sampling site, soil profiles were dug to 100 cm depth. The soil profiles were characterised based on AD-HOC-AG Boden (2005) and soil samples analysed for soil organic carbon (SOC), total nitrogen (N), total inorganic carbon (TIC), rock fragment content, texture, pH_{H_2O} (soil:water = 1:5), bulk density and electric conductivity (soil:water = 1:5). Soil profiles were described per soil horizon, while composite soil samples for laboratory analysis were taken at fixed depth intervals (0–10, 10–30, 30–50, 50–70 and 70–100 cm). If a horizon boundary was at least 5 cm above or below a sampling depth boundary, an additional soil sample was taken. This allowed laboratory and field data to be merged. Based on chapter 2, the following properties were assumed to restrict root growth: (i) consolidated, non-diggable bedrock, (ii) rock fragment contents > 75 vol.-%, (iii) cementation (ortstein or other cemented soil structure), (iv) compactness (packing densities $> 1.75\,g\,cm^{-3}$), (v) sandy subsoil (> 95 % sand in > 30 cm depth), (vi) anoxia (reducing soil horizon), and (vii) acidity ($pH_{H_2O} < 5$). In sites with at least one RRL, potential rooting was classified as restricted, while at those sites without any RRL rooting it was regarded as not restricted.

4.2.2 Adapting to root-restricting soil layers

To assess the adaptation of land use to RRLs, the grassland fraction of agricultural land was calculated per cause of root restriction (acidity, anoxia, sandy subsoil, compactness, cementation, rock fragments, bedrock or none) and each fraction compared to the total grassland fraction independent of RRLs. Grassland was defined as agricultural land that has been used as such for at least five consecutive years (EU, 2013). Then the study looked specifically at cropland and compared crop types on sites with RRLs to those on sites without RRLs. This comparison was based on the share of $crop_i$ in the crop rotation, i.e., the sum of years each site was used for $crop_i$ divided by the total number of reported site years (up to ten), where $crop_i$ represents one of the five most common crop types: winter wheat (*Triticum aestivum* L.), maize (*Zea mays* L.), winter barley (*Hordeum vul-*

gare L.), canola (*Brassica napus* L.) and winter rye (*Secale cereale* L.). Information on site-specific land use and crop rotations was derived from farmer questionnaires.

4.2.3 Meliorating root-restricting layers physically or chemically

Sites were identified that have been physically (drainage, deep chiselling or deep ploughing) or chemically (liming) meliorated, and the extent examined to which the observed melioration measures were explained by site-specific soil properties, geology, geography, land use and other management practices. A detailed overview of the explanatory variables used to predict soil melioration is presented in Table C.1. Information on physical and chemical site meliorations were primarily derived from farmer questionnaires. Drainage was defined as the anthropogenic removal of excess water from soil profiles via either pipe or trench drains. Deep chiselling was defined as in chapter 5 as an annual or irregular form of tillage, which aims to loosen (and not flip or mix) soil to greater depths than annual ploughing or, in cases where cropland was not ploughed, to > 30 cm depth. Fields were counted as deep chiselled if there was at least one documented deep chiselling event in ten years prior to sampling. If farmers did not provide data on the exact year of chiselling, it was assumed that this occurred also in the ten years prior to sampling (4 % of deep chiselled fields). Deep ploughing was defined as a single or irregular (not annual) ploughing treatment, which flips soil layers to greater depths than the normal depth of annual tillage (average depth 31 ± 0.1 cm) with the aim of subsoil melioration (chapter 5). At 29 % of deep ploughed sites, the year of deep ploughing was dated (oldest: 1934; youngest: 2015; average year: 1988), at 15 % of deep ploughed sites farmers were not sure about the year of deep ploughing, and at the remaining 56 % of deep ploughed sites, farmers were not aware that the site which they managed was once deep ploughed (historic deep ploughing only identified by soil profile descriptions). Liming was defined as the application of calcium-rich and/or magnesium-rich materials at least once in the ten years prior to sampling. If melioration data were not available in the questionnaires, an attempt was made to fill the respective gaps with information from site and profile descriptions from the field workers. However, in the case of drainage and liming, some gaps remained, leaving 85 % and 87 % of all sites for evaluation, respectively. The extent to which observed melioration measures could be explained with the variables listed in Table C.1 was examined using Random Forest models (Breiman, 2001). For each melioration measure (drainage, deep chiselling, deep ploughing and liming), one Random Forest Classification model was trained. Each model was trained to predict the probability of melioration at a given site. Probabilities $> 50\,\%$ were classified as meliorated and probabilities $\leq 50\,\%$ as not meliorated. The accuracy of each model (classifier) was assessed using tenfold cross-validation with random fold assignments. A comparison of predicted and observed classes produced four possible outcomes: (i) sites were correctly classified as meliorated (true positives), (ii) sites were correctly classified as not meliorated (true negatives), (iii) sites were falsely classified as meliorated (false positive), or (iv) sites were falsely classified as not meliorated (false negative). Based on these four possible outcomes, sensitivity (= true positive rate, hit rate or recall) and specificity metrics were calculated as follows: sensitivity = true positive/(true positive+false negative) and specificity = true negative/(true negative+false positive). Additionally, for each classifier, the area under its corresponding receiver operating characteristics (ROC) curve was calculated as implemented in the caret package (Kuhn, 2018). ROC curves depict trade-offs between the sensitivity and specificity of classifiers (Fawcett, 2006). The area under an ROC curve (AUC) provides a robust metric that can be used to compare the overall performance of classifiers (Kuhn & Johnson, 2013). In theory, AUC values can range from 0 (false prediction in all cases) to 1 (correct prediction in all cases). In practice, AUC values typically range between 0.5 (random guess) to 1 (correct prediction of all cases). In the original dataset, all melioration measures were imbalanced, i.e., the number of meliorated and not meliorated sites differed. Such class imbalances can have a strong negative impact on model fitting (Kuhn & Johnson, 2013). In this study, subsampling of the training data was applied within cross-validation resampling as implemented in the caret package (Kuhn, 2018) to overcome class imbalances. The following subsampling techniques were tested and evaluated against classifiers built without subsampling: down-sampling, up-sampling and two hybrid methods (ROSE by Menardi & Torelli (2014) and SMOTE by Chawla et al. (2002)). Based on the AUC, subsampling increased the performance of all melioration classifiers significantly, with down-sampling performing best, i.e., producing the highest AUC values. Therefore, all melioration classifiers discussed below were built using down-sampling.

4.2.4 Biopore abundance

Biopores were defined according to Kautz (2015) as continuous, round-shaped soil voids formed by plant roots and anecic earthworms. In the German Agricultural Soil Inventory, the abundance of root and earthworm channels was recorded separately at profile walls following AD-HOC-AG Boden (2005). Ordinal abundance classes recorded for each soil horizon were converted to a continuous scale using conversion factors (detailed description in Supplementary Material). As field workers who collected biopore data reported difficulties in separating root channels from earthworm burrows, the abundances of root channels and earthworm burrows were summed and evaluated together as biopores. Biopore abundance in 30–50 cm, 50–70 cm, 70–100 cm and 30–100 cm (total) was predicted using Random Forest Regression models based on all features listed in Table C.1. Like the binary classifiers described in the previous section, the biopore model was also evaluated using cross-validation. However, folds were not chosen at random but per field worker. In total, eight different field workers covered 89 % of all sites. Thus, the dataset was divided into 8 + 1 (for all other field workers) = 9 folds. Each fold covered between 235 and 651 sites. This target-oriented cross-validation was chosen in order to account for potential bias in evaluating biopore data collected by different field workers. To evaluate the accuracy of the biopore model, its root mean square error (RMSE) and coefficients of determination (R^2) based on target-oriented cross-validation were reported. AUC was not suitable for evaluating the biopore model because the former is only applicable for classification and not for regression problems.

4.2.5 Statistics

Data analysis was conducted in RStudio v 1.1.456 (RStudio Team, 2019) and R v 3.5.1 (R Core Team, 2018). To build Random Forest models (classification and regression), the `caret::train` function (Kuhn, 2018) was used in combination with `party::cforest` (Hothorn et al., 2005; Strobl et al., 2008, 2007). Each Random Forest model consisted of 500 trees and the mtry-parameter was set to the square root of the number of predictor variables (Hastie et al., 2009). Variable importance was calculated in accordance with (Breiman, 2001). Those variables of greater importance than expected from a theoretical model where all variables are equally important were considered influential (Hobley et al., 2015). The effect of influential explanatory variables on targets was illustrated using partial depend-

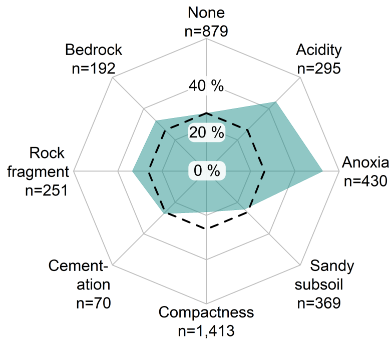


Figure 4.2: Grassland fraction of total agricultural land (green polygon) per root-restricting property. The dashed line illustrates the proportion of grassland from total agricultural land (26 %). If the green polygon is outside the dashed circle, grassland use is higher than on average agricultural soils. "n" gives the total number of sites per root-restricting property.

ence plots, which were computed using the `pdp::partial` function (Greenwell, 2017). Spider charts were created with `fmsb::radarchart` (Nakazawa, 2018) and all other figures using `ggplot2` (Wickham, 2016).

4.3 Results

4.3.1 Adaptation to root restrictions

Sites with root restrictions due to anoxia, acidity, rock content and/or bedrock were preferentially used as grassland (Fig. 4.2). Preferential grassland use was particularly pronounced at sites with anoxic subsoils due to groundwater or low pH values, where grassland use was 100 % and 69 % above the national average respectively. At sites with sandy subsoils and/or cemented soil structure, the proportion of grassland was similar to the national average. On agricultural land with root restrictions attributed to compactness, grassland use was below average.

Crop rotations differed significantly depending on the nature of RRLs (Fig. 4.3). On sandy, cemented, acidic and/or anoxic sites, the share of winter wheat was 36–70 % lower than on average croplands in Germany. Instead of winter wheat, farmers often chose to grow maize: maize cultivation was 61–105 % above average on sandy, cemented, acidic and/or anoxic sites. On cropland with shallow bedrock and/or high rock fragment contents, maize and winter rye were under-represented, while winter barley and canola were more common than on average croplands. In contrast, winter rye was largely over-represented on sites with sandy subsoils, cemented and/or acid soil layers.

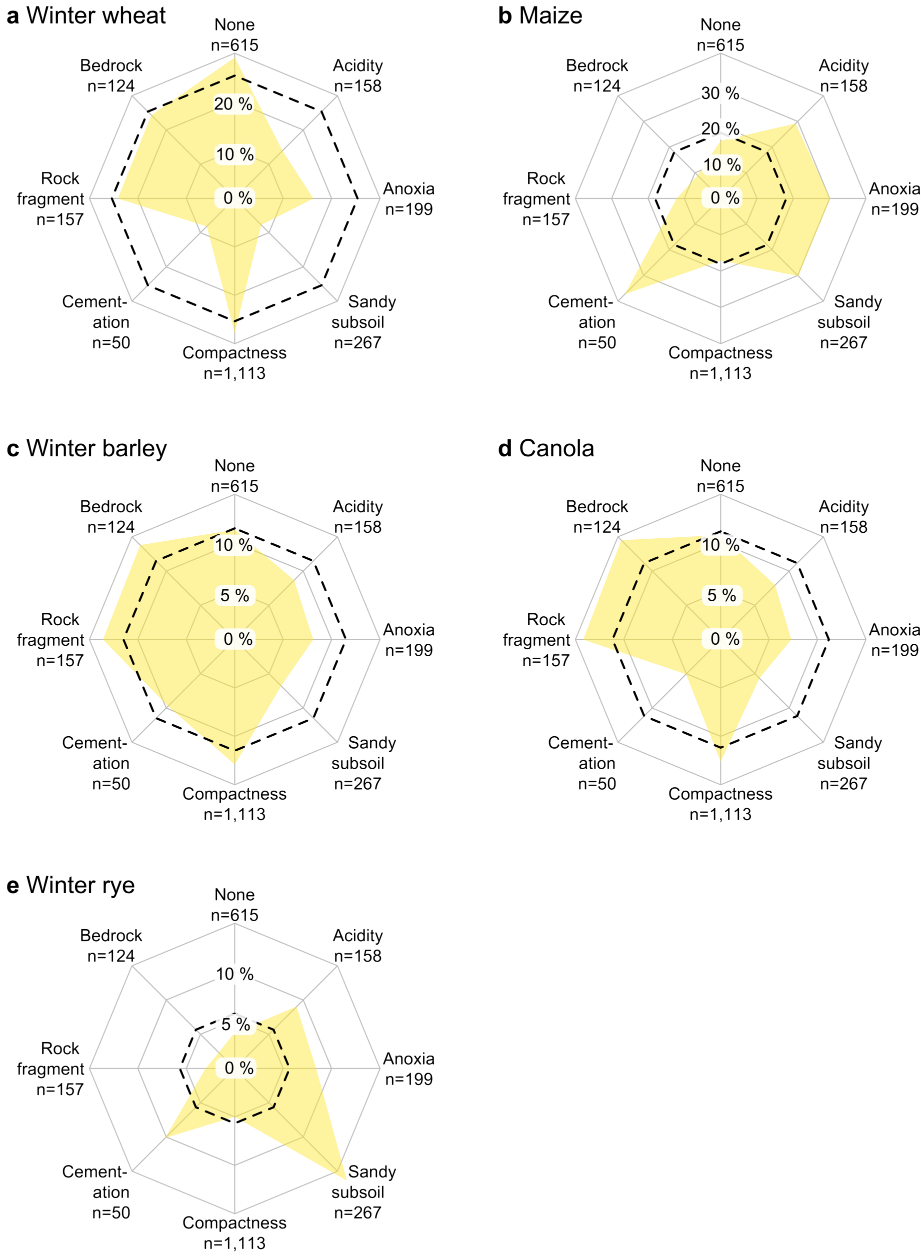


Figure 4.3: Share of the five most common crop types in crop rotations per root-restricting property (yellow polygons). Dashed lines illustrate the share of a given crop in crop rotations of all sites – independent of root-restricting properties. If the yellow polygon is outside the dashed circle, the abundance of a given crop is higher than on average agricultural soils. "n" gives the total number of sites per root-restricting property.

4.3.2 Physical and chemical melioration of root-restricting layers

Liming was the most popular management option examined in this study, with 54 % of sites being limed (Fig. 4.4). Liming probabilities were predicted with high accuracy (AUC = 0.84). Land use was the most important feature in predicting the likelihood of liming. About 66 % of cropland was limed. The likelihood of liming increased with the share of canola, sugar beet and/or leguminous crops in rotations. In grassland, liming was much less common than in cropland. Only 22 % of grassland was limed. The presence of geogenic or pedogenic carbonates decreased the likelihood of liming by half. In carbonate-free soil, regional differences were more important in explaining lime applications than soil pH. Liming was particularly common in northern Germany (latitude), where agricultural soil contained less clay and showed lower electrical conductivities than in southern Germany, which had less frequent liming. Hence, administrative and soil climate regions were also important in explaining lime applications.

After liming, drainage was the second most popular management option examined in this study, with 45 % of sites being drained. Machine learning performed well in predicting the likelihood of drainage (AUC = 0.83; Fig. 4.4). In contrast to liming, drainage was independent of land use. Instead, the degree of anoxia (reductomorphic features, depth of groundwater table, stagnogleyic horizon, semi-terrestrial soil order) and relict anoxia (oximorphic features) were most important in predicting the likelihood of drainage. Waterlogged soils occurred mostly in northern Germany, hence the classifier considered administrative regions (Lower Saxony, Schleswig Holstein, Mecklenburg Western Pomerania) and latitude (north) as important for predicting the likelihood of drainage. Drainage was preferentially performed at sites with morainic soil parent material, low slopes and large field size located in lowlands (geomorphology). Different causes of waterlogging, i.e., groundwater (Lower Saxony, coastline along the North Sea) or stagnant water (coastline along the Baltic Sea, Saxony, central southern Germany), were only of minor importance in explaining drainage. In total, 63 % of Gleysols and 69 % of Stagnosols under agricultural use were drained.

Deep chiselling was much less common within ten years prior to sampling (6 % of all sites) than liming or drainage activities. In contrast to the melioration measures described above, model performance was only moderate for deep chiselling (AUC = 0.73). As for liming, land use was the most important variable for explaining deep chiselling. Most (99 %) deep chiselling was conducted on cropland.

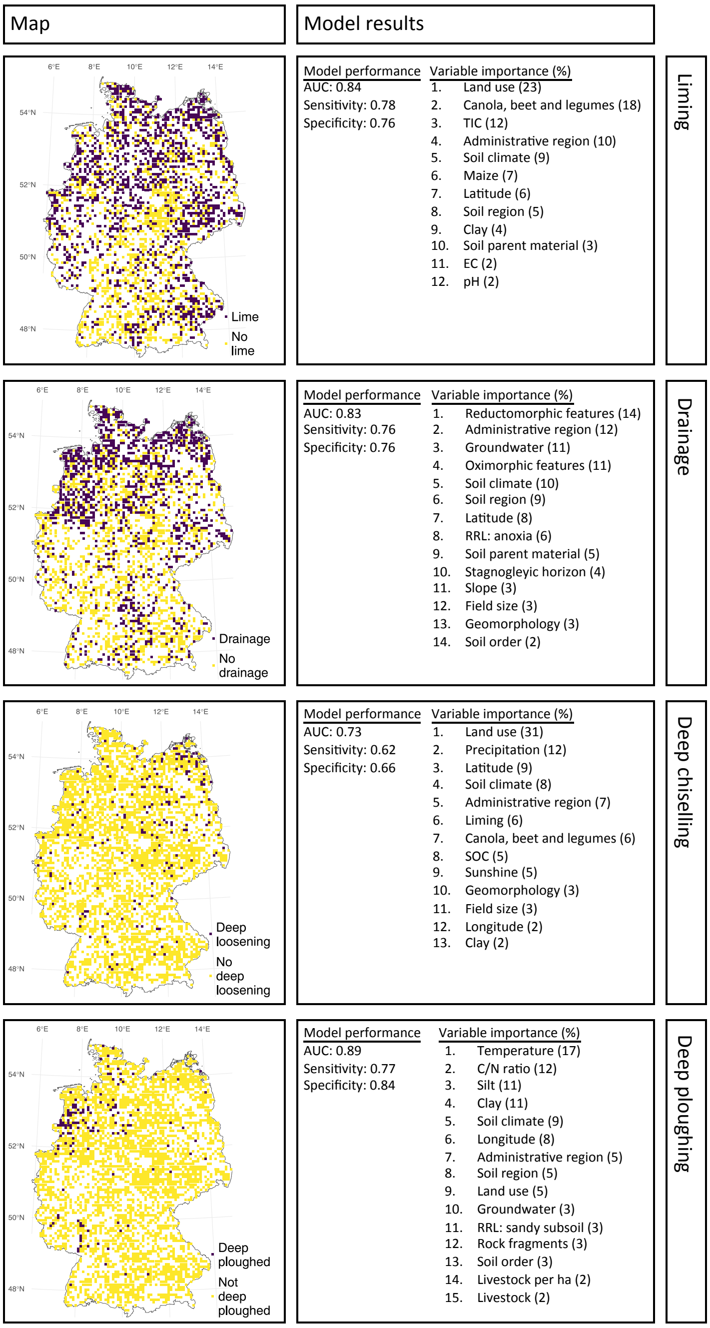


Figure 4.4: Physical and chemical melioration of German agricultural land. Left: Map of soil melioration measures documented in the German Agricultural Soil Inventory. Right: Performance and variable importance of Random Forest models trained to predict the likelihood of soil melioration. Model performances were characterised by (i) the area under the curve (AUC) metric, which may range from 0.5 (random guess) to 1 (perfect fit), (ii) the number of correctly predicted meliorated sites divided by the total number of meliorated sites (sensitivity), and (iii) the number of correctly predicted non-meliorated sites divided by the total number of non-meliorated sites (specificity).

Eight percent of annual crops and 15 % of perennial crops were deep chiselled. It was slightly more popular in eastern Germany, hence the likelihood of deep chiselling depended on administrative regions and other features that differed between eastern and western Germany: mean annual precipitation (low), sunshine duration (high), clay and SOC contents (both low) and field size (large). Furthermore, deep chiselling was preferentially conducted at sites that were flat and received regular lime applications.
About 5 % of agricultural soils were deep-ploughed at least once before sampling. Deep-ploughed sites were clustered mostly in northwest Germany and to a minor extent in viticultural areas along the valleys of the Rhine (between Karlsruhe and Mainz) and Mosel (between Trier and Koblenz). In northwest Germany, most deep-ploughed sites showed high C/N ratios, high sand contents, low rock contents and high groundwater tables. Furthermore, deep-ploughed sites in northwest Germany were characterized by relatively mild winter temperatures and high animal stocking rates. Deep ploughing by land use followed the order permanent crops (30 %), annual crops (4 %) and grassland (3 %). The relatively high share of deep-ploughed soil under permanent crops was due to the popularity of deep ploughing in the viticulture of the Rhineland Palatinate. The Random Forest algorithm grasped these patterns well and predicted deep ploughing with the greatest accuracy of all melioration measures examined in this study (AUC = 0.89).

4.3.3 Biopores

Biopores composed on average about 2.3 ± 0.04, 1.7 ± 0.03 and 1.1 ± 0.03 vol-% of the soil matrix in 30–50, 50–70, and 70–100 cm depth respectively. However, there were significant regional differences related to physicochemical soil properties (Fig. 4.5, Fig. C.3). Most biopores were found along the coast of the Baltic Sea, in the loess belt of central Germany, and in the alpine foreland south of the Danube river. In sandy soils, which cover large parts of Lower Saxony and Brandenburg, no or few biopores occurred. The Random Forest model trained to predict biopore densities of subsoils performed relatively poor: R^2 ranged from 0.16 to 0.22 depending on depth increments (Fig. 4.6). This can likely be attributed to considerable random error in the biopore estimates due to conversion from ordinal to continuous scale. Nonetheless, the model identified meaningful input variables as important. Silt content was most important for predicting the share of biopores: the more silt, the more biopores there were. Rock fragments, how-

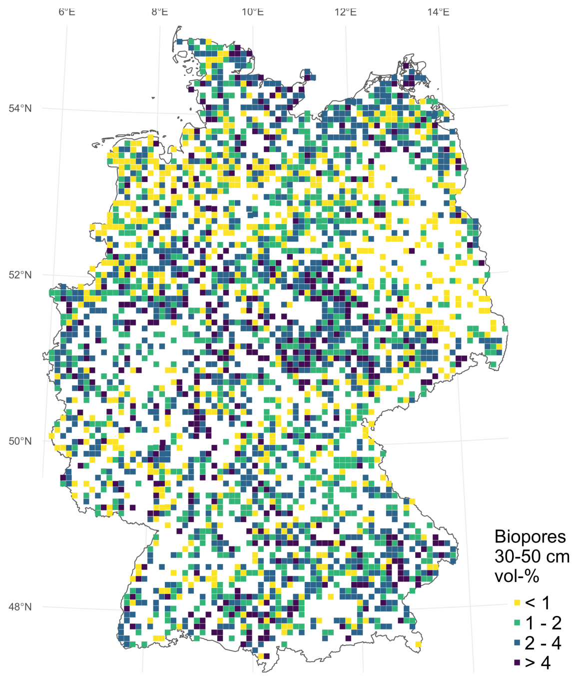


Figure 4.5: Biopore abundance in German agricultural soils at 30–50 cm depth.

ever, decreased the share of biopores in soils. Furthermore, biopore abundance increased with soil pH, clay content, SOC, C/N ratio (only in 30–50 cm depth) and increasingly dark soil colour, i.e., decreasing Munsell value (only in 50–100 cm depth). There was no evidence for land use effects on biopore abundance in subsoils.

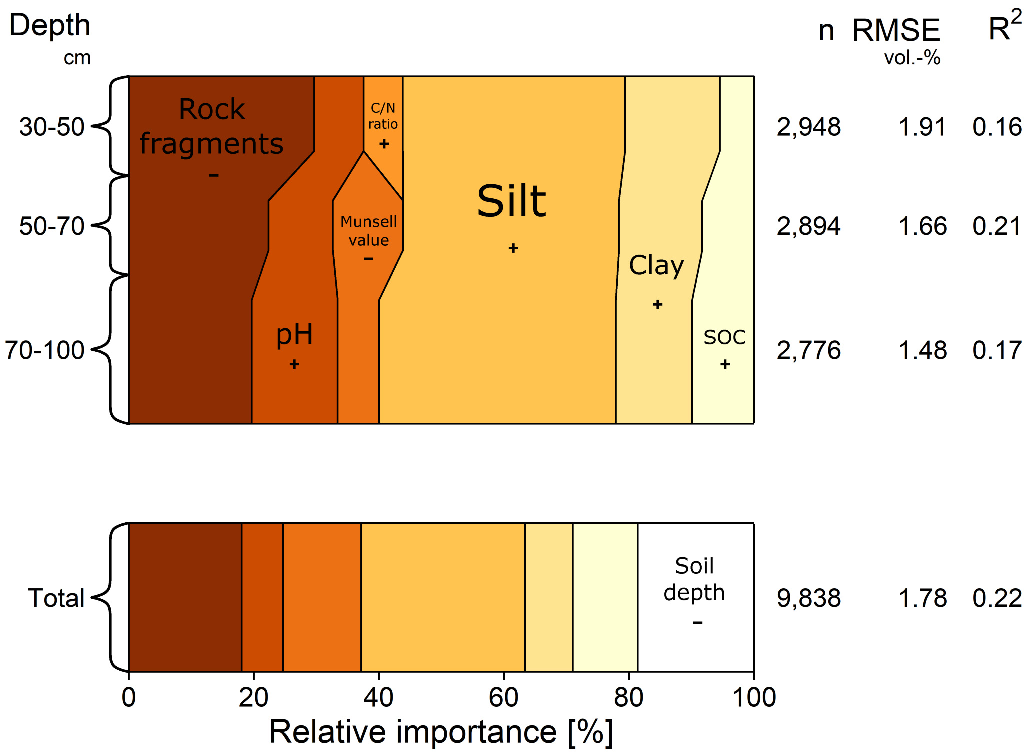


Figure 4.6: Significant predictors of the abundance of biopores in mineral soils by depth. Areas are proportional to the relative importance of the predictors. Each model is characterised by the number of observations in the training data ("n") and errors from tenfold cross-validation (root mean square error ("RMSE") and coefficients of determination ("R^2")). Positive marginal effects of continuous predictors on biopore abundance are illustrated as "+" and negative effects as "-".

4.4 Discussion

4.4.1 Adaptation to root restrictions

At sites with RRLs due to anoxia, acidity, rock fragments and shallow bedrock, grassland use was above average. However, this preferential grassland use might be explained by lower yield potentials due to RRLs (chapter 2). Nevertheless, the workability of soil has to be considered when discussing the effect of soil quality on land use. Diepolder et al. (2014) attributed preferential grassland use of Gleysols to challenges in trafficking soils with high groundwater tables. Rock fragments hinder tillage practices and the preparation of seedbeds, while shallow bedrock can render ploughing impossible. However soil quality is just one of many factors influencing land use. Land use is also governed by socioeconomic drivers such as market demand, subsidies, infrastructure, alternative livelihoods to farming and demography (van Vliet et al., 2015). Such socioeconomic drivers might explain why on sites with lower yield potential due to sandy or cemented soil layers, land use did not differ from the national average. On compacted sites, grassland use was below average. This can be explained by cropland use-induced soil compaction (chapter 2), and not vice versa. Moreover, most productive cropland soils with a high silt content (Luvisols) are also prone to subsoil compaction due to pedogenic lessivation.
In cropland with RRLs due to sandy subsoils, high groundwater tables, acidity and/or cementation, winter wheat and canola were under-represented, while maize and winter rye were over-represented (Fig. 4.3). This is in line with the typical requirements of these crops (Goldhofer et al., 2014a). Rye is generally regarded as the least demanding cereal crop planted in Germany with respect to pedogenic and climatic stressors (Goldhofer et al., 2014b). Rye tolerates acidic soil and periodically stagnant water much better than winter wheat and canola. Furthermore, rye typically roots relatively deeply, which makes it more drought-tolerant in sandy soil than wheat (Goldhofer et al., 2014b). The pedological niche of maize is similar to that of rye (Goldhofer et al., 2014b).

4.4.2 Physical and chemical melioration of root-restricting layers

Liming was the most popular melioration option examined in this study. However, in order to meliorate soils with root restrictions due to pH values < 5 (10 % of all sites), future lime quantities should exceed current application rates (Jacobs et al., 2018). As the surface application of lime may take years to leach through the soil column (Tang et al., 2003), amelioration of acid subsoils can be increased by applying more soluble gypsum minerals (Shainberg et al., 1989). Lime could also be applied directly in the subsoil if combined with deep chiselling. Such deep placements of lime in loosened furrows have been shown to typically reach only $< 20\,\%$ of the subsoil volume (Schmid et al., 1972). Despite the distribution problem of lime in subsoils, Richard et al. (1995) reported a positive crop yield response to deep placements of lime in compacted and acidic subsoil. During the German Agricultural Soil Inventory, no evidence was found of deep placements of lime. However, liming popularity depended strongly on land use: although soil under grassland tends to be more acidic than under cropland use, only relatively few grasslands (22 %) were limed. This is in agreement with farmer extension services who recommend lower pH values for grassland than for cropland (Wendland et al., 2014).

Drainage proved to be a highly popular measure in meliorating both Gleysols (lowering the groundwater table) and Stagnosols (drainage of stagnant water). Characterising the degree of anoxia was of primary importance for predicting the likelihood of drainage, which occurred mostly in anoxic soils. This might seem contradictory since successful drainage decreases the degree of anoxia, and not vice versa. However, the following two reasons can explain the positive correlation between the degree of anoxia and likelihood of drainage: (i) drainage is performed only at sites with high degrees of anoxia, and (ii) to predict the likelihood of drainage, the degree of anoxia down to 1 m depth was characterised but most farmers drain their land to < 1 m depth (Patt & Gonsowski, 2011). Drainage to 40-80 cm is sufficient to allow grazing (Diepolder et al., 2014) and draining to 80–100 cm for trafficking on cropland (Patt & Gonsowski, 2011). Yield losses attributed to anoxia (chapter 2) do not seem to justify the cost of draining agricultural land more deeply.

Deep chiselling was slightly more common in eastern Germany than in western Germany. This can partially be explained historically because in the former German Democratic Republic, subsoil melioration techniques were promoted on a large scale (Lindner et al., 1972; Renger, 1974). However, todays farm structures may also favour deep chiselling activities in eastern Germany. Since German Reunification in 1990, most agricultural production cooperatives have been privatised (BMWi, 2018; Wilson, 1996) and today most agricultural land belongs to large farms that generate relatively high revenues (BMEL, 2017). Considering the high costs of deep chiselling, todays farmers in eastern Germany might be more willing to adopt deep chiselling due to their greater financial power. Climatic factors can also be used to explain the popularity of deep tillage in eastern Germany: soil needs to be sufficiently dry during deep chiselling in order to shatter and not smear, and eastern Germany tends to be drier than western Germany. When predicting the likelihood of melioration, it was interesting that the model for deep chiselling performed worse (lower AUC value) than models for other physico-chemical melioration measures. This indicates that, apart from environmental and socioeconomic (field sizes, farm size and type etc.) features, farmer idiosyncrasy (family traditions and individual beliefs) plays an important role in the adoption of deep chiselling practices.

About 5 % of German agricultural land has been deep ploughed at least once in history. Considering that many of todays landowners are highly sceptical about deep ploughing (Frelih-Larsen et al., 2018), this share seems relatively large. Many deep-ploughed sites are clustered in northwest Germany close to the Dutch-German border. Most of them are a legacy of the "Emslandplan" – a land reclamation act that was passed by the German parliament shortly after the Second World War with the goal of converting heathland and peatland in northwest Germany into agricultural land (Eggelsmann, 1979). This was achieved by draining the peatland, then partly excavating the peat and finally deep ploughing. Massive steam engines were used to deep plough the remaining organic layer and the Podzol soil underneath down to 2 m depth with the goal of (i) improving drainage by shattering cemented ironpans (ortstein), and (ii) mixing the organic layer with sand to improve the trafficability and workability of the affected sites (Eggelsmann, 1979). High C/N ratios and a sandy soil texture were key parameters for predicting deep ploughing. This confirms that most deep-ploughed sites were former heathland or peatlands. Apart from northwest Germany, deep-ploughed sites were also clustered in wine-growing regions along the Rhine and Mosel. In German viticulture, deep manual digging (> 50 cm) was performed for centuries (Mollenhauer, 2014). Since the start of industrialisation, viticultural soil is often deep ploughed when renewing vineyards (Coulouma et al., 2006). Apart from viticulture, deep ploughing is rarely practised on agricultural land in Germany today.

4.4.3 Biopores

Compacted soil can be meliorated biologically by increasing the number of biopores. This can only be achieved indirectly, either by increasing the number of anecic earthworms or by including plant species with large taproots in crop rotations. Earthworm abundance in cropland has been shown to depend on aeration, texture and pH, with the highest abundances observed in well-aerated soils of silty texture and pH values from 5 to 7.4 (Curry, 2004). Alfalfa (*Medicago sativa* L.) and other taprooted crops, which have been promoted for biopore-enhancing management (Han et al., 2015b), require similar growing conditions as earthworms (Hartmann et al., 2014). Physicochemical soil properties, which provide optimal growing conditions for anecic earthworms and taprooted plants, can also benefit the structural stability of biopores. In well-aerated loess soils, relict earthworm burrows have been shown to be stable for decades or even centuries (Don et al., 2008). In non-loess soil, biopore stability might be much lower. In extremely sandy soils, burrows might collapse faster than in silt due to low adhesion forces among sand particles (Schrader & Zhang, 1997). In heavy clay soils, seasonal shrinking and swelling of clay minerals could potentially have a negative impact on biopore stability. Well-aerated soils also show no stagnant water or groundwater that could induce the collapse of biopores (Bottinelli et al., 2010). Hence, biopore abundance should be highest in non-acidic, well-aerated loess soils because they provide optimal environments for biopore formation and stability. This is in perfect agreement with the results obtained in the present study. These results confirmed that biopore abundance is closely linked to soil texture and pH. Furthermore, the results suggest a positive correlation between biopores and SOC. Increased SOC levels could be earthworm-derived, e.g., in the form of burrow linings (Don et al., 2008), but also root-derived and resulting from increased litter inputs in biopore-containing soils. Enhanced rooting might also explain the relatively wide C/N ratio, which correlates with biopore abundance in 30–50 cm depth. Finally, there could be positive feedbacks between rooting, biopore formation and SOC contents. Anecic earthworms are highly responsive to inputs of fresh litter (Curry, 2004). Decaying plant roots could provide such litter and stimulate earthworm burrowing along with SOC accumulation.

Land use had no effect on biopores in subsoils. This was surprising since the abundance of anecic earthworms is typically much higher in grassland than in cropland (Spurgeon et al., 2013). It is hypothesised that in cropland, the absence of

biopore formation by earthworms is compensated for by taprooted crops such as canola (*Brassica napus* L.). Field workers reported that canola formed biopores that were used preferentially by roots of subsequent cereal crops to grow into the subsoil (Schemschat, Bernd; pers. communication). In recent decades, the area under canola has risen from $< 0.1\,\%$ of German cropland in the 1950s to $11\,\%$ in 2016 (Destatis, 2019; Goldhofer et al., 2014a). The rising popularity of canola may have led to increased biopore formation in cropland. However, this remains speculative since in the present study there were no data on the origin and age of the biopores, hence it was not possible to distinguish between earthworm-derived and taproot-derived biopores. The absence of effects of land use on biopore abundance could also be explained by the dependence of land use on soil types and associated stabilities of biopores. Anoxic soils with high groundwater tables and low biopore stability were preferentially used as grassland (Fig. 4.2), while on loess soils with high biopore stability grassland use was negligible and cropland dominated.
To the best of our knowledge, the German Agricultural Soil Inventory is the first inventory to provide information on biopores in agricultural soils at national scale. Large observation numbers allowed biopore data to be evaluated and trends elucidated despite the fact that biopore abundance was only estimated visually by soil scientists. The regional clustering of biopores based on soil types suggests that successful melioration of densely-packed soil layers by means of biopores is restricted to loamy soils with high amounts of silt and little sand, low rock fragment contents, pH values > 5 and well-aerated sites.

4.4.4 Prespectives

Subsoils offer tremendous stocks of water and nutrients for plants. In the past, many efforts have been made to improve the plant availability of these resources. However, data derived from the German Agricultural Soil Survey suggests that at more than half of German agricultural land access to subsoil remains restricted (chapter 2). This hampers agricultural productivity already today and, considering alarming climate change scenarios, is likely to limit the former even more in the future. Upcoming management of agricultural land with RRLs should be based upon the wealth of past experiences. Positive effects of deep tillage on yield, which were observed in previous research trials (chapter 5), were often not confirmed in practice because of traffic-induced recompaction of mechanically loosened soil. Mixing loosened subsoil with organic materials may stabilize the disturbed soil structure and improve the plant-availability of subsoil resources on the long term (Jayawardane et al., 1995). For German agricultural land, potential benefits (productivity, carbon sequestration etc) and hazards (nitrate leaching etc) of furrow-wise loosening and deep mixing of organic matter are currently examined within the Soil^3 project[1]. Cultivation of alfalfa and other tap-rooted crops provide a biological alternative to mechanical deep tillage and can improve the plant-availability of water and nutrients in compacted subsoils. This has long been known but the current share alfalfa in crop rotations is only minor because economic barriers limit its uptake (Frelih-Larsen et al., 2018). Financial incentives could help to overcome these barriers.

4.5 Conclusions

Melioration has been carried out on 73 % of German agricultural soils in order to improve plant-growing conditions. In most cases, it was not only aimed at facilitating deeper rooting, but also at improving infiltration (deep tillage), aeration (drainage), nutrient availability (liming of acid soils) as well as workability and trafficability (drainage). Compacted plough pans can be meliorated by deep chiselling if the soil is dry enough. However, as shown in chapter 2, soil compactness was most severe at the maximum sampling depth of 70–100 cm. Below 50 cm, mechanical deep chiselling is barely effective, but biopores could still enhance rooting. Generally, biopore-promoting management can be recommended for all except sandy, acid, anoxic and gravelly soils. Deep ploughing used to be a popular technique to break up ironpans in Podzols. Today, the area extent of German agricultural soils with ironpans is negligible and the use of deep ploughing is restricted to viticultural areas. The relatively large proportion of German agricultural land with permanently anoxic subsoils due to high groundwater tables could be meliorated by improved drainage, while extreme soil acidity could be meliorated by improved liming practices. However, in view of the costs of installing and maintaining drainage systems (especially in lowlands with a high groundwater table and little slope) and costs of liming, many farmers prefer to adapt to impaired growing conditions by using land extensively (i.e., as grassland). On sites with shallow bedrocks and/or high rock fragment contents, grassland use is often the only management option possible.

[1] `https://www.bonares.de/soil3` (last accessed May 29th 2020)

Chapter 5

Effect of deep tillage on crop yield

Adapted from
Schneider, F., Don, A., Hennings, I., Schmittmann, O., & Seidel, S. J. (2017). The effect of deep tillage on crop yield – What do we really know? Soil & Tillage Research, 174:193-204.

5.1 Introduction

Agriculture is facing new challenges due to climate change (Sillmann et al., 2013) and imminent supply shortages of nutrients (Cooper et al., 2011). This creates a need to access new nutrient and water sources. In cropland, the subsoil, i.e., the soil layer below the regularly tilled topsoil, can store almost 50 % of total nitrogen stocks (Wiesmeier et al., 2013) and 25–70 % of total phosphorus stocks (Kautz et al., 2013) and can retain water even under drought conditions (Kirkegaard et al., 2007). However, the availability of these resources to crops varies.
High soil strength often limits root propagation and thus the plant-availability of resources in the subsoil (Bengough et al., 2011). Subsoil strength tends to be naturally high because of the weight of the above soil column and internal frictional forces (Gao et al., 2016). Particularly dense soil layers of mostly pedogenic (e.g., clay illuviation, hardpan of Podzols) and, to a lesser extent, geogenic origin (e.g., soils with abrupt textural change in fluvial or tidal sediment deposits) often pose additional natural barriers for root growth. However, high soil strength can also be man-made (Batey, 2009). About 15% of the agricultural land in Europe is compacted by agricultural mismanagement (Oldeman et al., 1991). The ability of roots to propagate at high soil strength differs between crop types. Dicotyledonous annual crops tend to have thicker roots and therefore higher ability to propagate

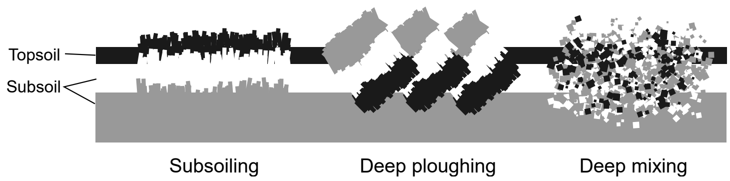


Figure 5.1: Schematic drawing of deep tillage-induced changes in the soil profile.

at high soil strength than monocotyledonous annual crops (Clark & Barraclough, 1999). In addition, dicotyledonous crops can improve the biopore network in the soil profile and build highways to the subsoil for subsequent crops (Kautz et al., 2013). However, today's annual cropping systems are vastly dominated by cereals and other crops with thin, fibrous roots. In soils without extensive vertical macropore channels or fissures, access to subsoil resources is thus restricted.
Mechanical modifications of soil profiles, commonly referred to as deep tillage, could alleviate high subsoil strength, facilitating deeper rooting and, thus, the plant availability of subsoil resources. Various deep tillage methods have been developed, including subsoiling, deep ploughing and complete mixing of soil profiles. Subsoiling aims at loosening the soil structure and decreasing the bulk density of the subsoil without turning or mixing soil horizons (Fig. 5.1, left). Subsoiling is sometimes referred to as deep ripping or deep chiselling. In contrast, deep ploughing turns soil horizons and results in complete or semi-complete inversion of the soil profile, with subsoil horizons ending up at the soil surface and topsoil horizons buried in the deep soil (Fig. 5.1, centre). Finally, there are deep tillage options that mix subsoil and topsoil, leading to complete destruction of soil horizons (Fig. 5.1, right). In the following, we refer to the latter management options as "deep mixing", in order to distinguish them from mere deep ploughing (turning) or subsoiling (loosening). Deep mixing can be conducted on the whole field (e.g., with a deep rotary hoe) or in stripes with undisturbed soil in between (e.g., with a wheel-type trencher).

The notion of improving the plant availability of water and nutrients from the subsoil by deep tillage has a long history. In pre-industrial times, soil was mostly tilled with animal-drawn ploughs, which rarely tilled deeper than 20 cm (Eggelsmann, 1979), and only manual digging was able to modify the soil profile to greater depths, like the labour-intensive method of double or triple digging. However, the latter was popular in confined areas only, e.g., in central European viticulture (Mollenhauer, 2014). Between 1850 and 1960, the development of steam and combustion engines allowed the maximum ploughing depth to be increased from 20 cm to ¿200 cm (Römer, 1940; Eggelsmann, 1979). The increase in horsepower and potential tillage depth enabled reclamation of peatland by deep ploughing on a large scale in northern Germany and the Netherlands. Furthermore, large areas of Podzols, Luvisols and Stagnosols were deep-tilled in order to decrease subsoil strength. In Germany alone, more than 500,000 ha were deep tilled to break up hardpans and loosen dense illuvial clay layers (Table D.1).

In the 1970s, the popularity of deep tillage declined among both the research community and practitioners. This was presumably largely due to inconsistent yield responses to deep tillage, which failed to compensate for the high execution costs. Concerns about negative effects of ploughing on beneficial soil biota (Kladivko, 2001) also increased general resistance to the use of tillage, especially among organic farmers. Within conventional arable farming, pesticides and herbicides supported the emergence of minimum tillage systems. However, chemical pest and weed control is not the primary goal of deep tillage. The mechanical modification of the subsoil as achieved by deep tillage can disrupt root-restricting soil layers and enhance water storage, improving soil fertility in the long-term (e.g., Schröder & Schulte-Karring, 1984; Baumhardt et al., 2008). With respect to soil biota, it is important to note that deep tillage can be either performed once for ameliorative purposes, i.e., with the goal of long-lasting improvements at a given site, or annually in order to achieve gradual topsoil deepening over time. Ameliorative deep tillage may have much less negative impacts on earthworms and other beneficial soil organisms than annual deep tillage (Kladivko, 2001). In several cases, ameliorative deep tillage has even been reported to enhance earthworm activities (Borchert, 1981; Fenner et al., 1993) and increase the abundance of plant growth-promoting rhizobacteria and mycorrhizae in the subsoil (Egerszegi, 1959; Müller & Rauhe, 1959; Steinbrenner & Naglitsch, 1965).

Inconsistent yield responses to deep tillage seem to occur at different sites and with different environmental conditions (Eck & Unger, 1985). Under drought stress, deep tillage could facilitate the uptake of subsoil water and thus stabilise crop yields (e.g., Doty et al., 1975). Climate change scenarios predict an increase in the intensity and frequency of droughts in many cropping regions of the world (Olesen et al., 2011; Porter et al., 2014). Deep tillage might be a tool to make crops more resilient to climate change and mitigate yield losses caused by droughts. Furthermore, because ameliorative deep ploughing of arable land sequesters carbon (Alcántara et al., 2016), deep ploughing carries the potential to compensate for greenhouse gas emissions and, if conducted on a large scale, may contribute to meeting future climate targets. Apart from climate change, limited access to fertilisers poses an imminent threat to crop production (Cooper et al., 2011). Subsoil nutrients have been shown to sustain yield in non-fertilised trials (Garz et al., 2000). Deep tillage might further enhance the plant availability of subsoil resources. However, a quantitative overview and understanding of crop responses to deep tillage is lacking to date (Olsson & Cockroft, 2006).

We therefore conducted an extensive quantitative review on deep tillage trials. Specifically, our goals were to (i) gain a quantitative overview of documented deep tillage effects on crop yield and (ii) examine the role of site-specific properties, management practices and drought stress in determining yield response to deep tillage. Data availability delimited the focus of our study primarily to short-term effects of deep tillage on the productivity of cereal crops grown on mineral soils in temperate latitudes.

5.2 Materials & Methods

5.2.1 General approach

We conducted an extensive review of studies about deep tillage effects on crop yield. Deep tillage was defined for each experiment, because tillage depth changed considerably during the observation period reviewed. In general, tillage treatments were defined as deep tillage if they reached deeper than in adjacent conventionally tilled control plots. Studies with repetitive deep tillage treatments were only considered if they examined gradual topsoil deepening and their initial experimental deep tillage treatment reached into the subsoil, i.e., soil which was not tilled before. Findings from organic soils like bogs and fens were excluded because of current environmental standards on peatland conservation.

Quantitative and qualitative methods were used for data evaluation. First, a meta-analysis of experimental field trials on deep tillage was performed. This delivered a quantitative overview of deep tillage effects on crop yield. However, highly variable reporting of experimental treatments and environmental conditions restricted identification and parameterisation of the forces driving deep tillage effects. Therefore, the meta-analysis was complemented with an extensive qualitative review of the literature. This qualitative review included studies that matched the criteria listed above and which described deep tillage-induced changes in soil fertility and/or crop yield. The procedure used for the meta-analysis is described in the following section.

5.2.2 Meta-analysis

Data collection

Web of Science was screened using the following keyword combinations: "yield" and "subsoil" with "tillage", "mixing", "ripping" or "ploughing"; "yield" with "deep ploughing", "subsoiling" or "deep ripping". Only articles written in English or German were considered. German literature was complemented with scientifically sound grey literature, mostly from the 1960s to 1980s because back then it was not common in German agricultural science to publish in international peer-reviewed journals. The search was confined to field experiments comparing the productivity of arable crops grown on ordinary-tilled control plots with adjacent deep-mixed, deep-ploughed or subsoiled plots, which apart from different tillage depths received the same treatments. Cases with subsoil fertilisation of deep-tilled plots were only included if the control plots received the same quality and quantity of fertiliser on the topsoil. Studies reporting extremely low grain or fresh matter yield (below 300 kg ha^{-1}) on either ordinary or deep-tilled plots in field studies with low or no fertiliser input, chemical pest control and replication were ignored, in order to keep the relevance for recent agriculture.

For each yield observation, information on site and management-related potential drivers was compiled. Explanatory variables were derived based on data availability (data given in as many studies as possible) and information content (continuous data better than categorical data). The resulting variables are listed in Table 5.1. Sites were classified based on the presence of root-restricting soil layers at deep tillage depth and their main textural class in the topsoil using the binary variables *RootRestrictingLayer*, *SandyTopsoil* and *SiltyTopsoil*. Sites classified with root-restricting soil layers featured either physical or chemical barriers to vertical root growth, which were either removed or disrupted by the deep tillage operation to 20 cm depth. Physical barriers included cemented layers (duripan and petroferric, gypsic or calcic horizons) and compacted hardpans of anthropogenic (plough pan) or natural origin (dense clay, fragipans). Chemical barriers were mostly due to anoxia in soil with stagnating water or groundwater and, in few cases, sodicity in saline soils. When the presence and depth of such root-

Table 5.1: Explanatory variables for modelling the effect of deep tillage on crop yield. Summary statistics are shown for the total dataset used to calculate the overall effect of deep tillage on crop yields (n = 1530) and for the subset without missing values used in regression analyses (n = 1471).

Explanatory variable	Type	Statistic & coding	Value		Unit	Explanation
			Total	Subset		
Site						
RootRestrictingLayer	B	0 = No root–restricting layer	1093	1086	–	Soils with hardpan, fragipan, duripan, plough pan, petrocalic, petrogypsic, petroferric, natric (Solonetz) or impermeable layer which was penetrated by deep tillage to > 20 cm depth.
		1 = Root–restricting layer	437	385		
SiltyTopsoil	B	0 = No silt	1143	1094	–	Topsoil was classified as silty for > 70% silt‡ and < 30% clay‡.
		1 = Silt	379	377		
		NA = not available	8	0		
SandyTopsoil	B	0 = No sand	870	822	–	Topsoil was classified as sandy for < 20% silt‡ and < 20% clay‡.
		1 = Sand	660	649		
Management						
TillageType	B	0 = Subsoiling	578	552	–	Type of tillage. We did not differentiate between deep ploughing and deep mixing because there were only few cases of deep mixing.
		1 = Deep ploughing& deep mixing	952	919		
TillageDepth	C	Range	4–134	4–134	cm	Difference between the deep tillage depth and control tillage depth.
		Median	20	20		
		Mean	23	22		
TillageFreq	C	0 = Not repeated	769	719	–	Average number of deep tillage interventions per site and per year.
		0.25 = Every 4th year	41	41		
		0.5 = Every 2nd year	284	284		
		1 = Annually	436	427		
FertiliserTop	B	0 = No topsoil fertilisation	384	384	–	Topsoil fertilisation on the control and deep tillage plots with mineral fertiliser or manure.
		1 = Topsoil fertilisation	1139	1087		
FertiliserDeep	B	0 = No subsoil fertilisation	1278	1226	–	Subsoil fertilisation on deep–tilled plots using mineral fertiliser, manure or plant residues. Cases were only included if there were adequate controls which received the same amount of fertiliser in the topsoil.
		1 = Subsoil fertilisation	245	245		
		NA = not available	7	0		
Time	C	Range	1–26	1–17	years	Number of years between the last deep tillage treatment and the recorded yield measurement.
		Median	1.5	1.5		
		Mean	1.8	1.7		
Water availability						
WaterQuantity	C	Range	0.9–8.7	0.9–8.7	mm (growing day)$^{-1}$	Sum of precipitation and irrigation water divided by the number of growing days (days between planting and harvest with TMIN > 0 °C).
		Median	2.3	2.3		
		Mean	2.3	2.3		
		NA = not available	52	0		
WaterIntensity	C	Range	3.2–22.5	3.2–22.5	mm (growing day with rain or irrigation)$^{-1}$	Sum of precipitation and irrigation water divided by the number of growing days with rain or irrigation (days between planting and harvest with TMIN > 0 °C and > 1 mm watering).
		Median	5.7	5.7		
		Mean	6.2	6.2		
		NA = not available	54	0		

B = Binary dummy variable; C = Continuous variable; TMIN = Daily minimum temperature.
‡ USDA soil texture classification.

restricting soil layers could not be judged based on the article concerned, a search was made for (i) other studies at the same site with more detailed soil descriptions and (ii) in the case of experimental sites in the USA, queries in the USDA NRCS Web Soil Survey database using reported or reconstructed coordinates of the sites (NRCS & USDA, 2013). If this search failed to provide an indication about root-restricting layers, soils were classified without such layers. Topsoil textural classes were derived from the same sources. Subsoil texture and other soil properties such as water regime and nutrient stocks could not be considered in the meta-analysis because of poor data availability.

Deep tillage methods were classified as subsoiling or deep ploughing and deep mixing (*TillageType*). The difference between the depth of deep tillage and conventional control tillage was recorded (*TillageDepth*). If the conventional control tillage depth was not explicitly stated, 20 cm was assumed for ploughing and 10 cm for all other control tillage types such as disking. Furthermore, the average number of deep tillage interventions per site and year was recorded, in order to characterise the frequency of deep tillage ($TillageFreq$). For each yield observation, we recorded whether the crop was fertilised and, if applicable, whether the fertiliser was placed on the topsoil ($FertiliserTop$) and/or in the subsoil ($FertiliserDeep$). Planting and harvesting dates were derived from the articles or, if not stated, from the crop and country (or US state) using specific average values presented by Sacks et al. (2010). The continuous variables $WaterQuantity$ and $WaterIntensity$ served as proxies for the seasonal availability of water. $WaterQuantity$ was calculated as:

$$WaterQuantity = \frac{\bar{P} + I}{n} \tag{5.1}$$

where $\bar{P}$ denotes cumulative precipitation during growing days (days between sowing or planting and harvesting with minimum temperature > 0 °C) in mm, I is the amount of additional irrigation water supplied in mm, and n is the number of growing days. Site-specific daily precipitation was calculated as the mean precipitation recorded by weather stations in a 100 km radius around each experimental field site, weighted by the reciprocal distance between each weather station and the field site. Daily minimum temperature was calculated following the same procedure. All precipitation and temperature records were downloaded from GHCN-Daily, Version 3.12 (Menne et al., 2012a,b). The irrigation inputs, I, were recorded from the articles. In general, water inputs per growing day varied considerably. Therefore, we created a variable for watering intensity, which was calculated as:

$$WaterIntensity = \frac{\bar{P} + I}{n_{\bar{P},I}} \tag{5.2}$$

where $n_{\bar{P},I}$ denotes the number of growing days with >1.0 mm precipitation and/or irrigation water input.

The dataset

Our search resulted in 1530 yield comparisons following deep and conventional control tillage on 67 experimental sites, which were extracted from 45 articles. The vast majority of the data derived from temperate latitudes and particularly from trials conducted in the USA and Germany, with 679 observations and 630 observations, respectively (Fig. 5.2). The dataset spanned a period of 105 years.

Of the total of 1530 observations, 437 (29 %) were derived from sites at which deep

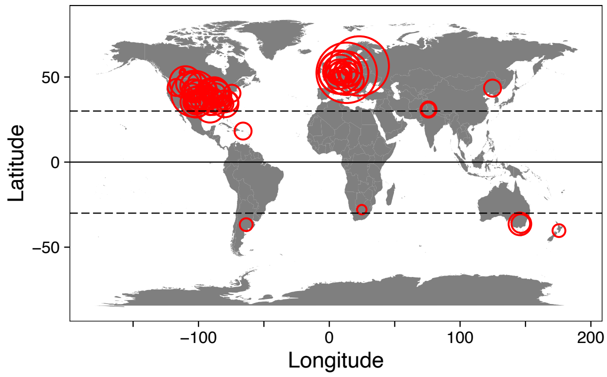


Figure 5.2: Locations of experimental sites included in this meta-analysis. Circle size increases with number of observations per site.

tillage disrupted root restricting soil layers (*RootRestrictingLayer*, Table 5.1). Root-restricting soil layers were mostly caused by dense clay layers (138 observations), followed by non-cemented plough pans and fragipans (65 observations), pans cemented by humic substances, gypsum, carbonate or iron (44 observations) and natric horizons (8 observations). In the remaining 138 observations, root-restricting soil layers were mentioned in the study, but their nature and cause was not further specified. Apart from root-restricting layers, experimental sites differed in topsoil texture. About 40 % of all observations derived from experimental sites with sandy topsoil and a further 25 % from sites with silty topsoil (*SandyTopsoil* and *SiltyTopsoil*; Table 5.1).

The deep tillage treatments consisted of subsoiling (578 observations), deep ploughing (779 observations) or deep mixing of the soil profile (173 observations) to 4–134 cm deeper (mean 23 cm) than in the conventionally tilled control plots (*TillageType* and *TillageDepth*; Table 5.1). The mean conventional control tillage depth was 19 cm. Around half the observations derived from ameliorative deep tillage trials in which the test site was deep-tilled only once (*TillageFreq*; Table 5.1). The other half derived from trials with repetitive deep tillage treatments every one to four years, with the goal of gradual topsoil deepening. The period between preceding deep tillage treatment and yield measurements was up to 26 years (Unger, 1993) (*Time*; Table 5.1). A quarter of all observations derived from field trials without mineral fertiliser or manure amendments. In 16 % of cases, deep tillage was combined with subsoil fertilisation and yield was compared with that in control plots with ordinary tillage and topsoil fertilisation.

Most trials were rain-fed, with only about 10 % of the observations deriving from irrigated crops. Considering both irrigation and precipitation, the crops received on average about 2.3 mm of water per growing day, ranging from 0.9 mm per growing day in Scottsbluff, NE, USA (Chilcott & Cole, 1918) to 8.7 mm per growing day in a heavily irrigated trial in Bushland, TX, USA (Hauser & Taylor, 1964). Watering intensity averaged 6 mm per growing day with rain and/or irrigation ($WaterIntensity$; Table 5.1).

Statistics

The effect size, i.e., the relative yield response to deep tillage, was calculated following standard procedures as:

$$ln(RY) = ln\left(\frac{Yield_{\text{Deep}}}{Yield_{\text{Control}}}\right) \tag{5.3}$$

where RY denotes the relative yield increase, which is defined as the ratio between the yield on the deep-tilled plot, $Yield_{\text{Deep}}$, and the yield of its respective control, $Yield_{\text{Control}}$, in the same unit (Rosenberg et al., 2013). Because indices for precision such as standard deviation or confidence interval were under-reported, each effect size was attributed the same weight. If not stated otherwise, differences were generally regarded as significant at $p < 0.1$. All statistical calculations were performed in R version 3.1.1 (R Core Team, 2016).
Effect size was modelled as a function of the predictors listed in Table 5.1 using ordinary least squares (OLS) and linear quantile regression (QR) analyses. While common OLS models estimate only the conditional mean response to some given values of predictors, QR allows any conditional quantile of the response distribution to be estimated (Koenker & Bassett, 1978; Cade & Noon, 2003). Here we used QR to evaluate the importance of the predictors in explaining positive and negative effect sizes. For predicting positive effect sizes, we ran a regression on the quantile Q of the conditional effect size distribution, which corresponded to a 15 % relative yield increase following deep tillage. This was at Q0.77, i.e., 77 % of the effect sizes were lower, while 23 % were higher. For predicting negative effect sizes, we ran a second regression on the quantile Q0.10 of the conditional effect size distribution as Q0.10 corresponded to a 15 % relative yield decrease following deep tillage. In the results and discussion section below, we use the regressions on the conditional quantiles Q0.77 and Q0.10 in order to illustrate and discuss the effect of the predictors on positive and negative deep tillage effects, respectively.

For completeness, in the appendix we present yield responses following deep tillage on further conditional quantiles (Q0.1 to Q0.9 in 0.1 increments; Fig. D.1).
For the regression analyses, 59 observations with missing values in any of the predictors were omitted, mostly due to unknown irrigation water inputs in irrigated trials. All continuous predictors except $TillageFreq$ were transformed by the natural logarithm to account for their large positive skewness. None of the explanatory variables was highly correlated ($r_s < 0.7$). Regression coefficients were calculated treating all observations as independent of each other. Clustering of the model residuals by studies suggested the presence of unobserved effects on study level, i.e., effect sizes reported in the same study tended to be similar. Compared with the differences between studies, differences between experimental sites within the same study were only minor. Therefore, robust standard errors were calculated from study-level cluster-bootstrapped simulations ($R = 2000$) for QR coefficients (Hagemann, 2016) and OLS regression coefficients (Fernihough, 2013). The resulting errors present conservative estimates which account for similar management and environmental factors driving observations from the same studies that could not be parameterised and fully captured by the explanatory variables available (Cameron & Miller, 2015). All QR coefficients and errors were calculated using the R quantreg-package (Koenker, 2016).

In a post-hoc analysis, the benefits of deep fertiliser placement were evaluated by examining only studies which included deep tillage treatments with and without subsoil fertilisation. The effect of subsoil fertilisation was evaluated as:

$$Deep\ fertilisation\ effect = ln\left(\frac{RY_{\text{``subsoil fert.''}}}{RY_{\text{``no subsoil fert.''}}}\right) \tag{5.4}$$

where $RY_{\text{``subsoil fert.''}}$ denotes the relative yield increase following deep tillage with subsoil fertilisation and $RY_{\text{``no subsoil fert.''}}$ denotes the relative yield increase following deep tillage without subsoil fertilisation but otherwise identical treatments. Differences between $RY_{\text{``subsoil fert.''}}$ and $RY_{\text{``no subsoil fert.''}}$ were assessed for each study separately using pair-wise Wilcoxon Signed-Rank tests.

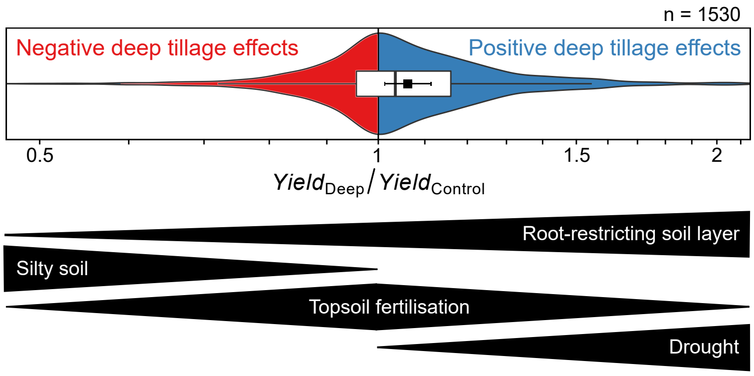


Figure 5.3: Deep tillage effects on crop yield. Top: Overall distribution (violin plot, box plot and mean ± 95 % confidence interval). Bottom: Significant drivers of yield response to deep tillage. The thicker the width of a horizontal bar, the more likely that the given condition was true.

5.3 Results & Discussion

5.3.1 Overall impact of deep tillage on yield

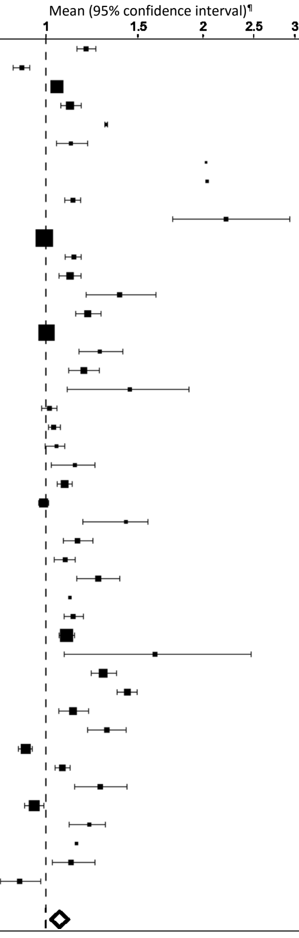
The mean crop response to deep tillage was significantly positive. Deep tillage increased yield by average 6 %, with a 95 % confidence interval around the mean ranging from 1 % to 11 % (Table 5.2). However, individual deep tillage effects were highly scattered (Fig. 5.3). Deep tillage increased yield only in about 60 % of the observations, while in the remaining 40 % of cases deep tillage resulted in yield depression. Studies reporting highly positive deep tillage effects were contradicted by many other studies documenting neutral or negative deep tillage effects (Table 5.2). To the best of our knowledge, this study is the first to provide a quantitative overview of the primary literature on the effect of deep tillage on crop yield. In the following section, we review and evaluate potential drivers of the different crop responses to deep tillage.

5.3.2 Drivers of deep tillage-induced changes in yield

Limitations of the meta-analysis

Data availability restricted the focus of our meta-analysis primarily to short-term effects of deep tillage on the productivity of cereal crops grown in temperate latitudes. Therefore, our findings should only be generalised within this framework and inferences beyond this should be made with care. The heavy skew towards short-term effects of deep tillage is partly explained by different experimental designs: about half the observations included in the meta-analysis derived from

Table 5.2: Studies included in this meta-analysis: Chilcott & Cole (1918); Smith (1925); Apsits (1935); Martinez & Lugo-López (1953); Opitz & Tamm (1953); Kohnke & Bertrand (1956); Anderson et al. (1958); Egerszegi (1959); Rauhe & Müller (1959); Larson et al. (1960); Rauhe (1960); Saveson et al. (1961); Hauser & Taylor (1964); Bowser & Cairns (1967); Schneider & Mathers (1970); Schulte-Karring (1970a); Weise (1970); Grass (1971); Mathers et al. (1971); Schnieder (1971); Rasmussen et al. (1972); Foerster (1974); Doty et al. (1975); Kamprath et al. (1979); Bradford & Blanchar (1980); Musick et al. (1981); Martincovic (1983); Chaudhary et al. (1985); Sene et al. (1985); Bennie & Botha (1986); Eck & Unger (1985); Ellington (1986); Ide et al. (1987); Bartels (1989); McAndrew & Malhi (1990); Unger (1993); Gajri et al. (1994); Allen et al. (1995); Frederick & Bauer (1996); Sojka et al. (1997); Varsa et al. (1997); Frederick et al. (1998); Motavalli et al. (2003); Botta et al. (2006); Cai et al. (2014).



Study	Country	Deep tillage type[†]	Crop[‡]	*Maximum period*[°] *[years]*	*Yield*$_{Deep}$/*Yield*$_{Control}$ Mean (95% confidence interval)[¶]		Obser-vations	Sites
Allen *et al.* (1995)	USA	P	Cereals	25	1.19	(1.15 - 1.24)	9	1
Anderson *et al.* (1958)	USA	S	Cereals	1	0.90	(0.87 - 0.93)	8	1
Apsits (1935)	LVA	PS	Cereals, Roots and tubers	1	1.05	(1.03 - 1.07)	140	1
Bartels (1989)	DEU	MPS	Cereals	11	1.11	(1.07 - 1.16)	42	1
Bennie and Botha (1986)	ZAF	S	Cereals	1	1.30		2	1
Botta *et al.* (2006)	ARG	S	O	2	1.12	(1.04 - 1.20)	4	1
Bowser and Cairns (1967)	CAN	P	Legumes	7	2.03		1	1
Bradford and Blanchar (1980)	USA	M	Cereals	1	2.04		2	1
Cai *et al.* (2014)	CHN	S	Cereals	1	1.13	(1.09 - 1.17)	8	1
Chaudhary *et al.* (1985)	IND	S	Cereals	1	2.21	(1.74 - 2.86)	7	1
Chilcott and Cole (1918)	USA	PS	Cereals, O	3	0.99	(0.97 - 1.02)	287	12
Doty *et al.* (1975)	USA	S	Cereals	1	1.13	(1.09 - 1.17)	8	1
Eck (1986)	USA	M	Cereals	17	1.11	(1.06 - 1.17)	32	1
Egerszegi (1959)	HUN	P	O	1	1.38	(1.19 - 1.61)	10	1
Ellington (1986)	AUS	S	Cereals	3	1.20	(1.14 - 1.27)	26	2
Foerster (1974)	DEU	MP	Cereals, Roots and tubers	6	1.00	(0.99 - 1.02)	243	5
Frederick and Bauer (1996)	USA	S	Cereals	1	1.27	(1.18 - 1.40)	4	1
Frederick *et al.* (1998)	USA	S	Legumes	1	1.18	(1.11 - 1.26)	24	1
Gajri *et al.* (1994)	IND	S	Cereals	1	1.45	(1.12 - 1.87)	5	1
Grass (1971)	DEU	PS	Cereals, O	4	1.02	(0.98 - 1.05)	8	1
Hauser and Taylor (1964)	USA	PS	Cereals	3	1.03	(1.01 - 1.06)	9	1
Ide *et al.* (1987)	BEL	S	O	3	1.05	(1.00 - 1.09)	3	1
Kamprath *et al.* (1979)	USA	S	Legumes	2	1.14	(1.04 - 1.24)	4	2
Kohnke and Bertrand (1956)	USA	S	Cereals, Legumes, O	1	1.09	(1.05 - 1.13)	36	2
Larson *et al.* (1960)	USA	S	Cereals	3	0.99	(0.97 - 1.01)	55	7
McAndrew and Malhi (1990)	CAN	P	Cereals, O	20	1.42	(1.18 - 1.57)	3	3
Martincovic (1983)	DEU	S	Cereals	2	1.15	(1.08 - 1.23)	12	2
Martinez and Lugo-López (1953)	PRI	S	O	1	1.09	(1.04 - 1.14)	8	1
Mathers *et al.* (1971)	USA	MP	Roots and tubers	2	1.26	(1.14 - 1.41)	17	1
Motavalli *et al.* (2003)	USA	S	Cereals	1	1.11		2	1
Musick *et al.* (1981)	USA	P	Cereals	13	1.13	(1.08 - 1.18)	9	1
Opitz and Tamm (1953)	DEU	P	Cereals, Roots and tubers, Legumes	1	1.10	(1.06 - 1.13)	145	1
Rasmussen *et al.* (1972)	USA	P	Cereals, Legumes	3	1.62	(1.12 - 2.61)	8	1
Rauhe (1960)	DEU	P	Cereals, Roots and tubers, Legumes, O	5	1.29	(1.22 - 1.36)	51	6
Rauhe and Muller (1959)	DEU	M	Cereals	2	1.43	(1.38 - 1.49)	24	1
Saveson *et al.* (1961)	USA	MPS	O	2	1.13	(1.06 - 1.21)	36	2
Schneider and Mathers (1970)	USA	P	Cereals	3	1.31	(1.21 - 1.42)	12	1
Schnieder (1971)	DEU	P	Cereals, Roots and tubers	10	0.92	(0.89 - 0.94)	72	1
Schulte-Karring (1970a)	DEU	S	Cereals, Roots and tubers	8	1.08	(1.04 - 1.11)	22	1
Sene *et al.* (1985)	USA	S	Cereals	1	1.27	(1.14 - 1.42)	12	1
Smith (1925)	USA	PS	Cereals, Legumes	4	0.95	(0.91 - 0.99)	91	2
Sojka *et al.* (1997)	NZL	PS	Cereals	1	1.21	(1.10 - 1.29)	4	1
Unger (1993)	USA	M	Cereals	26	1.14		2	1
Varsa *et al.* (1997)	USA	S	Cereals	4	1.12	(1.03 - 1.23)	12	1
Weise (1970)	DEU	P	Roots and tubers, Legumes	3	0.89	(0.81 - 0.98)	11	1
TOTAL					**1.06**	**(1.01 – 1.11)**	**1530**	**67**

[†] S = Subsoiling; P = Deep ploughing; M = Mixing
[‡] Cereals = Cereals; Roots and tubers = Roots and tubers; Legumes = Legumes; O = Other crops
[°] Maximum number of years between previous deep tillage operation and yield measurement
[¶] The size of squares is proportional to the observation number; confidence interval only shown if at least three observations per study

studies with recurring deep tillage treatments in at least every second year to achieve gradual topsoil deepening over time (mean period between yield measurement and preceding deep tillage 1.2 years; mean difference between tillage depth of control and deep tillage 16 cm). The other half of the observations described the effect of non-recurring, usually more intense, deep tillage interventions with the goal of long-term soil improvement (mean period between yield measurement and preceding deep tillage 2.7 years; mean difference between tillage depth of control and deep tillage 31 cm). Among the 26 studies examining long-term effects of non-recurring, ameliorative deep tillage on yields, 20 (77 %) lasted for five years or less. This might be explained by the short duration of many research projects and the lack of long-term funding sources. Observations of long-term deep tillage effects mostly derived from studies without continuous yield records and field trials, which might only have been rediscovered and systematically studied because preceding visual observations were "promising", i.e., indicated more vigorous growth on the formerly deep-tilled plots. On the other hand, studies documenting long-term deep tillage effects may not have been conducted or published because long-term effects were negligible. Thus, publication bias may cause considerable overestimation of the average long-term effects of deep tillage on crop yield. In a long-term study on ameliorative subsoiling, soil physical properties have been shown to follow non-linear trends over time (Borchert & Graf, 1985). This further indicates that generalisation of our results to predict long-term effects of deep tillage on crop yield is tainted with high uncertainty.

Deep tillage has a long history in soil preparation for perennial crops such as grapevines, pome fruits and asparagus (Bechtle, 1985). This tradition seems to be based on the practical experience of generations of farmers, as substantiating experimental data are scarce. In this meta-analysis, the only study reporting observations for perennial crops was on sugar cane grown in Puerto Rico (Martinez & Lugo-López, 1953). Our dataset consisted almost entirely of observations on annual crops, with 1092 observations (74 %) on cereals, 228 (15 %) on roots and tubers, 69 (5 %) on legumes and 82 (6 %) on other crops. Because there were relatively few observations apart from cereals, crop-specific influences on yield responses to deep tillage could not be included in the analysis. Some researchers have reported less stunted growth and less rotting in sugar beet after deep tillage (Mathers et al., 1971; Ide et al., 1987). However, this effect could not be quantified and, if present, contributes little to average trends.

Finally, the dataset mostly comprised observations from temperate latitudes (Fig. 5.2).

In subtropical and tropical latitudes, higher solar radiation might compromise the usefulness of $WaterQuantity$ and $WaterIntensity$ as rough proxies for drought intensity because of considerably higher evapotranspiration rates. However, the magnitude of this effect remains speculative and was neglected in this study because the share of observations from the subtropics and tropics was negligible ($< 1\,\%$).
When modelling the large variation among individual effect sizes, it was a challenge to define suitable explanatory variables. Great variation among individual reporting styles resulted in a need to aggregate available information and create several dummy variables. Available predictors might only have been non-significant due to the limitations in parameterising driving forces. Thus, there is a need to place the results of the meta-analysis in a wider context. In the following sections, we embed the results of our meta-analysis in a qualitative review of the literature in order to discuss the driving forces of different crop responses to deep tillage.

Site-specific effects

The success of deep tillage depends strongly on site-specific conditions. The meta-analysis revealed that root-restricting layers were the most important driver for positive crop yield responses to deep tillage. On sites with root-restricting soil layers, deep tillage effects were generally 20 % higher than at sites without such layers (Fig. 5.4, *RootRestrictingLayer*). This difference was highly significant ($p < 0.001$). Thus, deep tillage can destroy barriers to vertical root growth and facilitate uptake of growth-limiting resources from the subsoil. The resources stored in the subsoil contribute significantly to crop performance (Kuhlmann et al., 1989; Kirkegaard et al., 2007; Kautz et al., 2013). We therefore estimate that at least 20 % of the resources needed for cereal crop production in temperate latitudes derive from the subsoil. This is a conservative estimate, as root-restricting layers are usually not positioned at but below the boundary between topsoil and subsoil.

Soil texture is another key variable for crop response to deep tillage. At sites with silty topsoil ($> 70\,\%$ silt), negative deep tillage effects on crop yield were significantly more frequent and severe than at sites with less silty topsoil. This is illustrated by the negative QR regression coefficient of $SiltyTopsoil$ for negative effect sizes (Fig. 5.4B). Our meta-analysis thus suggests that intensive deep tillage should be restricted to soils low in silt. This conclusion is in line with studies examining the effect of deep tillage on soil physical properties. In an extensive

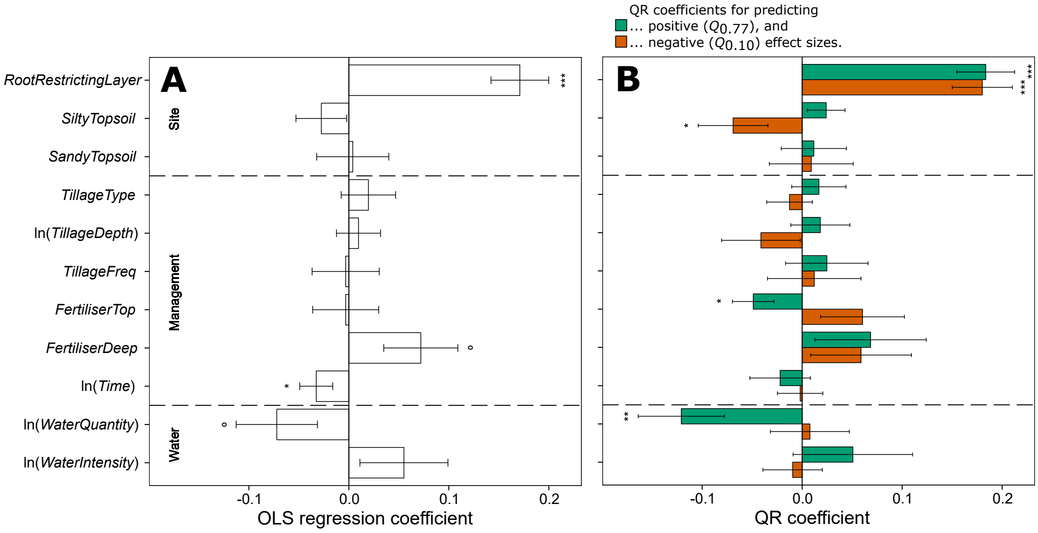


Figure 5.4: Effect of site, management practices and water availability on crop response to deep tillage. (A) Ordinary least squares (OLS) regression estimates predicting the conditional mean effect size. (B) Quantile regression (QR) estimates for positive and negative effect size. Error bars illustrate robust standard errors based on study-level clustered-bootstrap simulations. Significance is shown for coefficients with $p < 0.1$, 0.05, 0.01 and 0.001 with $\circ$, $*$, $**$ and $***$, respectively.

long-term field study conducted at 67 sites in south-east Germany, subsoiling only lowered the bulk density and increased the macroporosity of soil if it contained $> 20\,\%$ clay and $< 70\,\%$ silt (Borchert, 1975, 1981, 1984; Borchert & Graf, 1985). On many soils with a clay:silt ratio <0.3, subsoiling resulted in complete collapse of the natural soil structure and compaction instead of loosening. Management options to facilitate uptake of water and nutrients from the subsoil of silty loess soils with low clay content should therefore focus on biological options such as deep-rooting catch crops (Renger, 1974). This promotes the formation of long-term stable biopores, which can serve as highways for subsequent crop roots to access subsoil resources (Kautz et al., 2013). In silty, loamy and clayey soils, biopores seem to be important pathways for roots to access resources from the subsoil (Han et al., 2015b; Colombi et al., 2017). Deep tillage comes at the cost of destroying these biopores. On very silty soils, deep tillage has been shown to have little potential to loosen the soil matrix and to decrease the bulk density (Borchert & Graf, 1985; Müller, 1985). Along with the destruction of biopores, this might explain the increased likelihood of yield depression on deep-tilled silty soils observed in the present meta-analysis.

Sandy topsoil texture showed no significant effect on crop response to deep tillage (Fig. 5.4, *SandyTopsoil*). In contrast, Sene et al. (1985), who deep-loosened 12 sites with contrasting texture in the North Carolina Coastal Plain, USA, were able to explain 93 % of the variation in crop response by the sand content in the topsoil. Our results show that the distinction between sandy and non-sandy topsoil does not suffice to predict the success of deep tillage at many sites. In two studies included in this meta-analysis, yield decreased after deep tillage of sites with sandy topsoil (Weise, 1970; Schnieder, 1971). At both sites, only the topsoil was sandy, while the subsoil was loamy. Classifying the texture of subsoils into sandy or non-sandy might prove more constructive in predicting deep tillage effects on crop yield. However, this could not be evaluated in the present meta-analysis because in most studies included in the dataset subsoil texture was not specified. Very sandy subsoils often exhibit a single-grained, non-cohesive structure with few continuous biopores, which could facilitate root growth (Amelung et al., 2018). Thus, root elongation has to overcome the mechanical impendence of the soil matrix as well as frictional forces between sand grains and the roots (Bengough et al., 2011). In densely packed, sandy subsoil, high mechanical impendence and frictional forces can restrict root growth (Batey & McKenzie, 2006; Batey, 2009). Observations from Hungary and India suggest that deep tillage can loosen densely packed sand grains in the subsoil, thus decreasing mechanical impendence and facilitating root elongation through the loosened subsoil matrix and resulting in considerably larger crop yields in the following growing season (Egerszegi, 1959; Chaudhary et al., 1985). However, due to low data availability on subsoil texture, these effects reported for single sites could not be generally quantified.

Deep tillage methods

There is great variety among deep tillage methods. Based on data availability, in this meta-analysis we differentiated between deep tillage options (subsoiling vs. deep ploughing and deep mixing), tillage depths and tillage frequency. In doing so, we were unable to observe significant differences between tillage options (Fig. 5.4; *TillageType*). In the regression models, the disruption of a root-restricting soil layer by deep tillage was more important than details on how and how often it was disrupted (Fig. 5.4; *RootRestrictingLayer* vs. *TillageType*, ln(*TillageDepth*) and *TillageFreq*). However, this approach does not permit generalisation of the findings or predictions that different methods of deep tillage will result in the same crop response regardless of site and environmental conditions.

A qualitative review of the literature showed that deep tillage options should be designed to fit site-specific needs and constraints.

In general, the response of the soil to all deep tillage options is related to its water content. Successful deep tillage requires soil water content to be below the plastic limit from the topsoil to the maximum tillage depth (Borchert, 1975; Eck & Unger, 1985). The plastic limit is defined as the water content at which thin threads of soil rupture when rolled out (Atterberg, 1914; McBride, 2002). In addition to the water content, soil texture should also be considered. In soils with $> 40\,\%$ clay, the plastic limit is not reached until the permanent wilting point at -1.5 MPa (Renger & Strebel, 1976). In humid climates, such low soil matric potentials may rarely be reached. In a case study in north-west Germany, Renger & Strebel (1976) estimated that the plastic limit of heavy soils is only reached in about 1 to 3 out of 10 years. Heavy soils in humid climates can be prepared for deep tillage using water-consuming crops like alfalfa and by prior drainage (Schulte-Karring, 1985). As our climate is currently changing, increasing drought duration and intensity could increase the likelihood of soil reaching the plastic limit in some cropland regions (Dai et al., 2004). However, soil water content will remain a major constraint for successful deep tillage of heavy soils in humid climates. Nonetheless, in most studies reviewed, data specifying soil water content during deep tillage were either lacking or remained vague.

Subsoiling can be a successful tool to treat soils with physical barriers to root growth (Schulte-Karring, 1970a; Chaudhary et al., 1985; Schulte-Karring & Schröder, 1986; Gajri et al., 1994). The loosening effect of subsoiling mainly depends on the plasticity of the soil and the machinery used. Machines for subsoiling can be classified into lift-loosening and break-up loosening technologies (Schulte-Karring & Haubold-Rosar, 1993). Among lift-loosening technologies, machines with moving tines have been shown to be superior to those with fixed tines (Schulte-Karring, 1995). Loosening intensity generally increases with increasing subsoiling depth and decreasing distance between loosened furrows (Schulte-Karring, 1995; Spoor, 2006). Subsoiling of soils above the plastic limit, i.e., when too wet, may cause compaction, plastic deformation, smearing and mole drainage effects (Müller, 1985). Poor soil loosening due to high soil water might explain many neutral and negative crop responses to subsoiling, especially in early trials (Smith, 1925; Anderson et al., 1958; Larson et al., 1960). On the other hand, heavy soil should not be too dry but still be friable when deep loosening. Otherwise, the pulling resistance exerted by the loosening tines can be too high and soil loosening im-practical.

Deep ploughing or deep mixing have the highest potential to improve duplex soils with textural changes (Seibel, 1972; Allen et al., 1995; Baumhardt et al., 2008), sandy soils (Egerszegi, 1959; Rauhe & Müller, 1959) and Solonetz soils with sodic barriers to root growth (Tyurin et al., 1960; Bowser & Cairns, 1967; Rasmussen et al., 1972). On very sandy soils, organic matter-rich topsoil, which is buried by deep ploughing, can act as a barrier to infiltrating water and nutrient leaching. Thus, deep ploughing sandy soils can increase water and nutrient storage. Deep placement of organic amendments can further enhance this effect (Egerszegi, 1959; Rauhe, 1960). On sodic soils, with a higher Ca^{2+} to Na^{+} ratio in the subsoil than in the topsoil, crop responses to deep tillage are among the highest recorded (Rasmussen et al., 1972). Flipping the Ca^{2+}-rich subsoil and the Na^{+}-rich topsoil increases the flocculation of soil colloids, improves soil structure and increases infiltration rates (Tyurin et al., 1960; Bowser & Cairns, 1967; Rasmussen et al., 1972). In soil profiles with pronounced textural changes, both deep ploughing and deep mixing have been successfully applied for removing root-restricting layers and increasing plant-available water storage (Seibel, 1972; Allen et al., 1995; Baumhardt et al., 2008). However, the site-specific benefits of deep ploughing or mixing may come at the cost of topsoil deterioration. For example, subsoil clay lifted by deep ploughing may hinder trafficability and complicate seedbed preparation (Scheffer & Meyer, 1970). In such cases, liming with CaO can improve soil workability (Bechtle, 1985). The risk of poor trafficability is especially pronounced in the first years after deep ploughing and deep mixing. Perennial crops require less traffic, which may explain why deep ploughing and deep mixing have been successfully applied for centuries in the production of perennial crops (viticulture, pomiculture and asparagus cultivation), while in annual cropping systems such soil profile modifications are rarely applied in practice. Apart from workability, the burial of topsoil and its replacement with nutrient- and organic matter-poor substrate from the subsoil may be another constraint to deep ploughing and mixing (Scheffer & Meyer, 1970; Harrach et al., 1971). After turning or mixing topsoil and subsoil, management efforts should therefore be devoted to building up soil organic matter in the new topsoil. Organic manure and increased mineral fertilisation can mitigate initial yield depression (Renger, 1974; Rojahn, 1974).

Soil nutrients and fertilisation

The effect of deep tillage on nutrient availability is site- and management regime-specific. On the one hand, our meta-analysis suggests that deep tillage can improve the accessibility of nutrients from the subsoil, which increases crop yield if the nutrient availability in the topsoil is deficient. This is illustrated by significantly higher yield increases after deep tillage in unfertilised trials compared with trials with fertilised topsoil (Fig. 5.4B, negative QR regression coefficient of $FertiliserTop$ for positive effect sizes). On the other hand, a pronounced but non-significant trend towards more extreme yield depression in other unfertilised field experiments suggests that deep tillage can also decrease nutrient availability and depress yield (Fig. 5.4B, positive QR regression coefficient of $FertiliserTop$ for negative effect sizes). This might be explained by increased mineralisation of organically-bound nutrients and subsequent leaching due to higher water infiltration or topsoil deterioration resulting from deep ploughing or mixing (Weise, 1970; Bechtle, 1985). Overall, topsoil fertilisation buffered crop response to deep tillage, i.e., in unfertilised trials, positive and negative deep tillage effects on crop yield were more extreme.

In some trials, deep tillage was combined with subsoil fertilisation. As the root density of annual crops tends to increase in spots with high nutrient concentrations, subsoil fertilisation can stimulate deeper rooting (Lynch et al., 2012). Deeper rooting can stabilise the mechanically disrupted soil structure and supply crops with resources from the subsoil, which mitigates yield depression, especially when a resource in the topsoil becomes growth-limiting (Kohnke & Bertrand, 1956; Schulte-Karring, 1985). Indeed, in the present meta-analysis, yield tended to be higher if a given type and amount of fertiliser was incorporated into the subsoil rather than into the topsoil (Fig. 5.4A; $FertiliserDeep$). However, this relationship needs to be interpreted with caution, as the number of observations with subsoil fertilisation was relatively small (Table 5.1). Our meta-analysis included seven studies that compared deep tillage treatments with and without subsoil fertilisation. Three of these studies evaluated the effect of deep ploughing or manual digging combined with deep placement of organic manure on crop yield at sandy sites (Fig. 5.5; top), while four studies examined the effect of subsoiling combined with deep placement of mineral fertiliser on crop yield in heavy soils (Fig. 5.5; bottom). On sandy soils, deep placement of manure generally resulted in higher

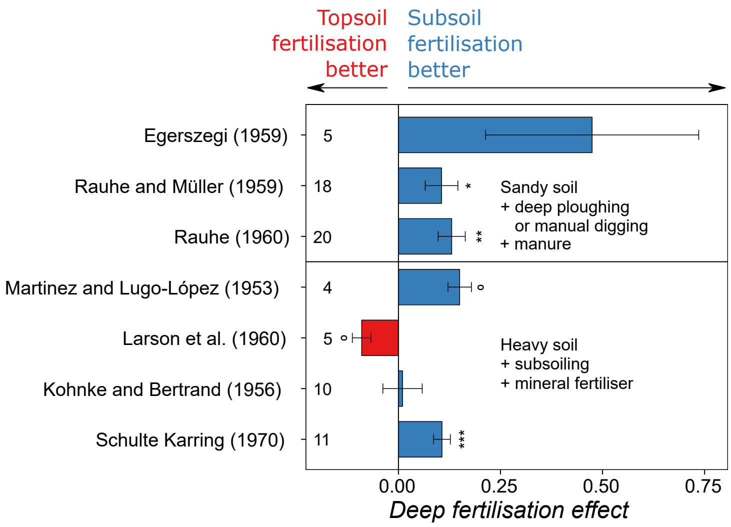


Figure 5.5: Effect of deep fertiliser placement, calculated as the difference between the relative yield increase following deep tillage + subsoil fertilisation and the relative yield increase following deep tillage alone grouped by study. In the case of subsoil fertilisation, yield observations with the same amount of fertiliser applied in the topsoil served as the control. Significant deep fertilisation effects following paired Wilcoxon Signed-Rank tests are shown for $p < 0.1$, 0.05, 0.01 and 0.001 with $\circ$, $*$, $**$ and $***$, respectively.

crop yield than incorporation of manure into the topsoil. The deep-placed manure stimulated deeper rooting and acted as a barrier to infiltrating water and leaching nutrients (Egerszegi, 1959; Rauhe & Müller, 1959; Rauhe, 1960). This increased yields and made crops much more resilient during droughts. The promising results of field trials contributed to the popularity and large-scale application of this technique in the former German Democratic Republic, where around 50,000 ha of sandy cropland was treated by deep ploughing combined with deep placement of manure or other organic amendments (Renger, 1974). However, the success of this method is restricted to deep sandy soils that are not underlain by finer-textured materials (Weise, 1970; Schnieder, 1971).

The results of mineral fertilisation of the subsoil on heavy soils were inconsistent (Fig. 5.5; bottom). On heavy soils, drought stress is less pronounced and deeper rooting might therefore be less beneficial than in light soils. Moreover, the stimulating effect on root growth depends on the composition of the mineral fertiliser. Larson et al. (1960) mostly injected only phosphorus into the subsoil and it generally stimulates root growth much less than nitrogen, which was used in other studies (Lynch et al., 2012). Finally, there are the technical constraints associated with the dispersal of fertiliser in the subsoil when the soil profile is only deeply loosened and not turned or mixed. Fertiliser that is placed or injected into the loosened furrow behind the subsoiling tines may only reach a maximum of 10–15 % of the total subsoil volume (Schmid et al., 1972). If the soil is moist during subsoiling, the dispersal of deep-placed fertiliser is even poorer due to the formation of fertiliser pockets. Preferential water flow in the loosened furrows may increase nutrient losses by leaching and increase the risk of eutrophication (Schmid et al., 1972).

Soil water

Our meta-analysis suggests that deep tillage increases the resilience of crops under drought stress. Positive deep tillage effects increased significantly with decreasing water inputs per growing day, i.e., drought intensity (Fig. 5.5; $\ln(WaterQuantity)$). The inverse relationship between water input and deep tillage effect was more pronounced at sites with root-restricting soil layers compared to sites without such layers (Fig. 5.6). This highlights the importance of the subsoil water reservoir for mitigating dry spells. The associated mechanisms can be manifold. On the one hand, deep tillage may increase the plant-available water pool by increasing the soil volume that is accessible to roots (Kohnke & Bertrand, 1956; Rauhe & Müller, 1959; Rauhe, 1960; Bowser & Cairns, 1967; Grass, 1971; Harrach et al., 1971; Mathers et al., 1971; Rasmussen et al., 1972; Rojahn, 1974; Doty et al., 1975; Kamprath et al., 1979; Bradford & Blanchar, 1980; Chaudhary et al., 1985; Bennie & Botha, 1986; Ide et al., 1987; Cai et al., 2014). On the other hand, deep tillage may increase the abundance of mesopores, which increases the capacity of soils to store plant-available water (Bartels, 1989). Finally, deep tillage may increase infiltration rates, reduce waterlogging and run-off, and thus increase water recharge (Martinez & Lugo-López, 1953; Kunze, 1963; Schneider & Mathers, 1970; Mathers et al., 1971; Schröder & Scharpenseel, 1975; Musick et al., 1981; Schulte-Karring & Schröder, 1983; Eck, 1986; Unger, 1993; Allen et al., 1995; Baumhardt et al., 2008). The latter point may also explain the amplifying effect of watering intensity on positive crop responses to deep tillage observed in our meta-analysis (Fig. 5.5B; $\ln(WaterIntensity)$). The more intense the watering event, the higher the difference between the water recharge and associated crop resilience between deep-tilled and conventionally tilled plots. However, this is speculative, as the effect of $\ln(WaterIntensity)$ was not significant. In the special case of deep ploughing sandy soils, the positive relationship between deep tillage effect and drought intensity may also derive from the known role of buried organic matter-rich topsoil as a barrier to infiltrating water (Renger, 1974). Our meta-analysis provides strong quantitative evidence of the potential of deep tillage in increasing the plant-available water reservoir and improving the resilience of crops in times of greater climate change-induced precipitation variability and extremes.

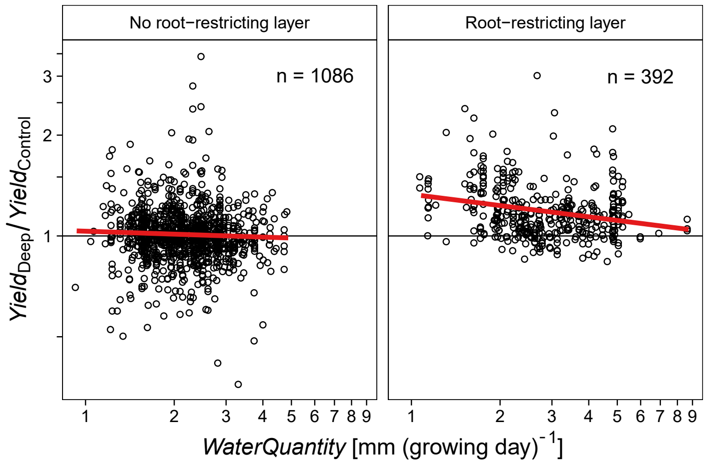


Figure 5.6: Water input per growing day plotted against the relative yield increase after deep tillage.

Deep tillage effects over time

The meta-analysis allowed few conclusions to be drawn about the persistence of deep tillage effects on crop yield. There was a slight trend towards decreasing benefits from deep tillage over time (Fig. 5.4A). Doubling the period between the preceding deep tillage treatment and yield measurement decreased effect size by on average about 2 %. However, the rate of this trend might have been highly underestimated, due to the peculiarities of our dataset described above.

Compaction of mechanically loosened soil has been shown to proceed faster on soils with > 70 % silt and < 20 % clay compared with soils with a higher clay content (Borchert, 1981). In soils with > 20 % clay, the mineralogy of clay seems to govern the rate of re-compaction in the following order: kaolinite > illite > smectite (Borchert, 1981). Traffic by agricultural machines further accelerates the rate of re-compaction (Czeratzki & Schulze, 1970; Schulte-Karring, 1970b; Grass, 1971; Ellington, 1986; Busscher & Sojka, 1987; Soane et al., 1987; Botta et al., 2006; Baumhardt et al., 2008). Sowing crops directly on top of loosened furrows or mixed trenches restricts subsequent vehicle passes to zones that were not deeply tilled, and thus prolongs the persistence of subsoiling and deep mixing effects (Sojka et al., 1993). If such in-row subsoiling or deep mixing is not possible, orthogonal vehicle passes over loosened furrows or slots are recommended (Schulte-Karring, 1985). Biological factors also play a key role in stabilising mechanically disrupted soil structure, e.g., by the extensive root system of catch crops and green manure (Schulte-Karring, 1985). Borchert & Graf (1985) attributed higher stabilisation of mechanically loosened soil structure to the abundance of annelids. Finally, the disrupted soil structure can be stabilised chemically by liming with CaO (Bechtle, 1985). This promotes flocculation of clays and the formation of clay-organic complexes. While the effect of mere subsoiling is estimated to decline over the course of a few years, deep ploughing and deep mixing may cause long-term changes in soil fertility.

5.4 Conclusions

Barriers that restrict annual crop roots from accessing the resources stored in the subsoil can cause severe yield depression. The adverse effects of such root-restricting soil layers are especially pronounced if the plant availability of nutrients and water in the topsoil is limited. Deep tillage can disrupt root-restricting soil layers and facilitate access to additional resources stored in the subsoil. Based on the present meta-analysis, we conclude that deep tillage has the highest potential to increase yield at sites with root-restricting soil layers in regions with erratic rainfall and pronounced dry spells. On sites without root-restricting soil layers, deep tillage effects on crop yields are inconsistent and may not be positive. Deep ploughing and mixing may warrant increased fertilisation and organic matter build-up during the first growing seasons to avoid yield depression due to topsoil burial. However, subsoiling does not carry this risk and may be a tool to increase nutrient availability in low input farming systems with nutrient-deficient topsoils. On soils with $> 70\,\%$ silt, all deep tillage activities carry an increased risk of imposing detrimental effects on crop growth.

Chapter 6

Final discussion

Subsoil is commonly perceived as the hidden part of soil that contains less roots, less organisms and less organic matter than the topsoil above[1]. In soil quality assessments, subsoil properties are often either valued negatively or not at all. Subsoils can be water-logged and therefore make fields not suitable for traffic or contain many rock fragments hindering the workability of soils. But what is subsoil good for? The value of subsoil is manifold and is differently perceived among disciplines. Archaeologists value subsoil for harbouring potential cultural heritage while craftsmen may appreciate subsoil clay as building material and for pottery. Biologists may value subsoil for providing a habitat to rare species and environmentalists for filtering toxic compounds as well as fertiliser from infiltrating water. In this thesis, I examined two further key functions of subsoil: (i) serving as a growing medium for plants and their roots, and (ii) storing organic carbon (C). To illustrate these functions, I first characterised site properties that restricted access of plant roots to subsoil and represented root-restricting soil layers (RRLs). Then, I examined how these RRLs affected crop yield and soil organic C storage. Finally, I discussed management options for agricultural soils with RRLs.

For the first time in history, the German Agricultural Soil Inventory has provided consistent and representative data about properties and management of agricultural soils in Germany (Fig. 1.1). In order to tap the full potential of this new dataset, I followed the suggestion of Kell & Oliver (2004) and complemented traditional hypothesis-driven research with inductive, data-driven research methods to work through the research questions of this thesis. In the following, I will first provide a brief summary of the key findings and then attempt to apply these findings for identifying promising target regions for subsoil management in Germany.

[1] See `https://de.wikipedia.org/wiki/Unterboden` (last accessed 12th May 2020)

6.1 Research questions

Which site properties impede root growth in German agricultural soils?

The dominant site property for restricted elongation of deep roots was high soil compactness. Almost half (46 %) of German agricultural land was compacted to an extent that restricted root growth. Other causes for restricted root growth were much less prevalent – their area relevance decreased in the following order: groundwater-induced anoxia (14 % of agricultural land), sandy subsoil texture (12 %), acidity (10 %), large rock fragment content (8 %), shallow bedrock (6 %), and cementation (2 %). The prevalence of RRLs differed significantly among soil groups. RRLs occurred in 91 % of all Podzol sites, in 89 % of Gleysols and in 82 % of Vertisols but only in 38 % of Chernozems. In Podzols, RRLs were mostly caused by sandy subsoil texture, cemented soil structure and/or acidity. In Gleysols, groundwater-induced anoxia restricted deep root growth. In Vertisols and Chernozems, most RRLs occurred due to high soil compactness.
The numbers cited above are based on a novel quantitative framework to classify the magnitude of root-restriction in temperate agricultural soils, which was developed in chapter 2. The framework distinguishes three levels of root restriction (none, moderate, severe) based on the criteria listed in Table 2.1. It was derived from a literature review and subsequently validated using root count data from the German Agricultural Soil Inventory. In 30–50 cm depth, relative root counts of winter wheat were 18 % lower in the presence of severe RRLs at or above 30–50 cm depth compared to reference soils without RRLs. In grassland, relative root counts were 32 % lower in the presence of severe RRLs at 30–50 cm depth. Moderate RRLs decreased relative root counts of winter wheat (grassland) only by 10 % (9 %) at 30–50 cm depth.

To what extent do RRLs limit the productivity function of agricultural soils?

Globally, RRLs decreased yield of annual crops on average by about 20 %. Generally, yield losses were most pronounced in growing seasons with droughts. In Germany, average grain yield of winter wheat (most common crop) was 6 % lower on sites with severe RRLs compared to reference sites without RRLs. On sites with moderate RRLs, grain yield of winter wheat was only 3 % lower.
These results confirm that RRLs limit the productivity function of agricultural soils, especially in growing seasons with droughts. The global estimate is based

on a meta-analysis of long-term field experiments, in which yield on sites with RRLs was compared with neighbouring sites that were meliorated by deep tillage (chapter 5). The national estimate for Germany was derived from data of the German Agricultural Soil Inventory (chapter 2). Winter cereals tend to be more drought tolerant than summer cereals (Goldhofer et al., 2014b), which might explain why the observed effect of RRLs on grain yield of winter wheat in Germany is lower than the global estimate. Also, the global estimate is based on experimental sites for which the magnitude of root-restriction could not be determined due to inconsistent reporting of data. It is possible that the experimental sites showed extremely severe magnitudes of root restriction, which inflated the global estimate.

Do RRLs limit the organic C storage function of agricultural soils?

The size of the soil organic C pool depends on organic C inputs to soil and organic C losses from soil. All RRLs limit root-derived C input into the subsoil. But some soil properties that restrict root growth (lower C input), may also increase C stabilisation (lower C loss), like the case for groundwater-induced anoxia (chapter 3). Therefore, generalising the net effect of root-restricting soil properties on soil organic C stocks is not straightforward.

In German agricultural soils, high compactness was by far the most dominant soil-borne cause for restricted rooting and compacted layers were associated with a significant drop in depth profiles of organic C densities. This suggests that compacted soil layers restricted C input more than they retarded C losses. Overall, compacted soil layers were estimated to have caused an average organic C deficit of 2.3 $Mg\,ha^{-1}$ in 30–100 cm depth (chapter 3). If all compacted layers were sustainably loosened, German cropland could store up to 0.03 Pg (4 %) more organic C in 30–100 cm depth.

Has anthropogenic soil compaction increased the spatial extent of RRLs in German agricultural soils?

The results of this thesis suggest that 37 % of the land, which is used as cropland today, is "naturally" compacted due to pedogenic causes[2]. Anthropogenic land use and management have increased this proportion to roughly 50 %. About

[2] Compacted soil is defined here as soil that restricts the potential of roots to elongate due to high compactness

10 % of cropland was compacted due to traffic, 1 % due to organic C loss-induced collapse of soil structure, and further 2 % due to a combination of both factors. Compaction caused by organic C loss was detectable down to 30 cm depth, whereas traffic-induced compaction was detected down to 50 cm depth. Most RRLs caused by anthropogenic compaction occurred directly below the plough layer, i.e., in 30–50 cm depth. In grassland, the effect of anthropogenic soil compaction on root growth was much less pronounced than in cropland and ranged below the detection limit.
In the literature, the spatial extent of anthropogenically compacted soil is highly debated. Uncertainties typically arise from (i) insufficient data to represent the target region of interest, (ii) separating pedogenic and anthropogenic causes of soil compactness, and/or (iii) threshold values to differentiate insignificant from harmful degrees of soil compactness. In the present thesis, uncertainty (i) was resolved by evaluating the recently completed German Agricultural Soil Inventory, which provides representative data for all agricultural soils in Germany. For quantifying anthropogenic effects on soil compactness (ii), a novel approach was developed (chapter 2):

train Random Forest model
to predict depth gradients of soil compactness
in non-compacted reference sites
⇓
use this model to predict soil compactness in target sites
⇓
compare measured compactness with predicted compactness in target sites

Concerning uncertainty (iii), in this thesis, root growth was assumed to be restricted in soil with packing densities above 1.75 g cm^{-3}, as proposed by the Joint Research Centre of the European Commission (Huber et al., 2008). This interactive web-graphic

`https://compact.shinyapps.io/play/`

illustrates how the here presented area estimates for compacted land would have changed if another threshold value was chosen. This calls for caution, when comparing area estimates for compacted soil from different sources.

How do farmers manage agricultural soils with RRLs in Germany?

German farmers either accept the presence of RRLs and adapt land use and management accordingly or they meliorate affected sites (chapter 5). Anoxic and acidic sites were preferentially used as grassland. Cropland with RRLs was often dominated by maize instead of wheat. The melioration measures differed depending on the cause of root-restriction. About 54 % of agricultural land in Germany was limed to correct soil acidity, 45 % was drained to remove excess water and improve aeration. About 6 % was deep chiselled at least once within ten years prior to sampling primarily to meliorate anthropogenic compaction. Finally, 5 % of agricultural soils have been deep-ploughed at least once in history, mostly to break cemented ironpans or loosen pedogenic hardpans. In German viticulture, deep soil loosening has a long tradition – it was already subject of proto-Romantic poetry[3] – and it is still widely practiced today before replanting vines.

In total, 73 % of German agricultural land have been meliorated in order to improve plant-growing conditions. However, it can be assumed that in most cases, site meliorations were not only aimed at facilitating deeper rooting, but also at improving infiltration (deep tillage), nutrient availability (liming of acid soil) as well as workability and trafficability (drainage). The German Agricultural Soil Inventory only recorded melioration measures but it did not inform about the success of the melioration measures. Therefore, a meta-analysis was conducted to examine the effect of deep tillage on crop yield in further detail (see below).

How does meliorative deep tillage affect crop yield?

Field studies on the effect of mechanical soil profile modifications, commonly referred to as meliorative deep tillage, on crop yield have delivered inconsistent findings. Therefore, (i) a meta-analysis about crop yield responses to subsoiling (loosening), deep ploughing (turning + loosening) and deep mixing of soil profiles was conducted, and (ii) relationships between site properties, management practices, water availability and deep tillage-induced changes in yield were reviewed. The meta-analysis was based on 1530 yield comparisons between deep and ordinary tillage at 67 experimental sites in mostly temperate latitudes. On average, deep tillage slightly increased yield (+6 %). However, the response of crops to deep tillage varied considerably among sites. Deep tillage increased yield only in about 60 % of the observations, while in the remaining 40 % of cases deep tillage

[3] See poem "Die Schatzgräber" by Gottfried August Bürger (1747-1794)

resulted in yield depression. At sites with RRLs, the crop yield response to deep tillage was 20 % higher than at sites without such layers. In general, differences between deep tillage methods were less important than the presence of RRLs. Soils with > 70 % silt (labile soil structure) showed an increased risk of negative deep tillage effects. In growing seasons with dry spells, positive deep tillage effects were greater than in average years. Topsoil fertilisation buffered both extremely positive and negative deep tillage effects. Overall, the results suggested that deep tillage increases the plant availability of subsoil nutrients, which increases crop yield if (i) nutrients are growth-limiting and (ii) deep tillage does not come at the cost of impaired topsoil fertility. On soils with stable soil structure and RRLs, deep tillage can be an effective measure to mitigate drought stress and improve the resilience of crops under climate change conditions.

6.2 Synthesis & Outlook

In the present thesis, both cause and extent of RRLs in German agricultural soils have been examined in detail. In the following, I will now derive a rough estimate concerning the amount of water and nutrient resources that are hidden below RRLs in German agricultural soils. Finally, I will discuss promising target regions for subsoil management to improve the plant-availability of these resources.

6.2.1 Hidden water and nutrients in subsoil

Plants are nourished by water and nutrients from the soil. If the plant-availability in one of these resources is limited, plants are stressed and decrease their productivity. But what characterises the plant-availability of a resource? Plant-availability is commonly defined based on the chemical or physical state, in which the resource is present in the soil – a plant-available resource is present in a from that can be readily assimilated by plants. In routine soil analyses, plant-available nutrient contents are estimated based on topsoil extractions that have been calibrated against the field response of crops to fertiliser (Marschner & Rengel, 2012). The plant-availability of water is typically determined in the laboratory by mimicking the suction force of plants. Such methods will reveal the proportion of the total water and total nutrient stocks, which are potentially plant-available. However, the potential plant-availability of a resource is also limited by its accessibility, which is often neglected. In topsoil, neglecting the accessibility constraint is legitimate in most cases since the rooting density in topsoil is typically high. In subsoil, however, the results of the present thesis suggest that the accessibility of a resource can be severely hampered. The larger the distance from the soil surface, the higher the metabolic cost for plants to incur the resource, and the higher the likelihood for encountering barriers that could increase these costs further or render access impossible (King et al., 2020). The present thesis revealed about 71% of German agricultural land to exhibit physical or chemical barriers for root growth (Table 2.1). Such RRLs limit the soil volume that is potentially available for rooting. Therefore, RRLs limit the potential plant-availability of water and nutrient resources for plant growth. In the following, I will estimate the amount of water and nutrient resources that are hidden below RRLs of German agricultural soils.

Methods. Water and nutrient resources in the upper metre of German agricultural soils were characterised from soil samples of the German Agricultural Soil Inventory. The magnitude of root restriction was defined according to Table 2.1. Only mineral soils, i.e., soil profiles that contained less than 87.2 $g\,kg^{-1}$ total organic C in all depth increments (AD-HOC-AG Boden, 2005), were considered because (i) the area extent of organic soil was minor (173 sites) compared to mineral soil (2931 sites), and (ii) organic soil did not serve as target for subsoil management (see section below).

Available water capacity served as an indicator for the water resource. It was calculated as the difference of water held in soil between field capacity (θ_{fc}, pressure head = −100 cm or pF 2.0) and the wilting point (θ_{wp}, pressure head = −15 800 cm or pF 4.2). θ_{fc} and θ_{wp} were estimated via pedo-transfer functions (PTFs) that required soil texture (FAO), bulk density, organic C content, and depth increment (topsoil or subsoil) as inputs. In total, three different PTFs from independent studies were applied. The first PTF was developed by Wösten et al. (1999) and was based on 5521 samples from Europe of which 2309 samples originated from Germany. The study of Wösten et al. (1999) was the most cited study when searching the Web of Science for “pedotransfer function” AND “soil” AND “water” (583 citations). The second PTF was calibrated on Belgium soil samples by Vereecken et al. (1989, 439 citations in the Web of Science) and recommended by AD-HOC-AG Boden (2004) for German soils. The third PTF was recently developed by Dobarco et al. (2019) specifically for French agricultural soils. The three PTFs yielded slightly different results with available water capacities in the upper metre showing an average standard deviation of 27 mm. Because validating the PTFs with own measurements was beyond the scope of this thesis, I decided to evaluate available water capacities on the basis of the mean value from the three PTFs in order to minimise systematic errors. Because none of the PTFs considered rock fragments, I corrected available water capacities as follows:

$$Available\ water\ capacity = (depth_{\text{lower}} - depth_{\text{upper}}) * \frac{\theta_{\text{fc}} - \theta_{\text{wp}}}{100} * \left(1 - \frac{rocks}{100}\right) \quad (6.1)$$

where *available water capacity* is given in mm, $depth_{\text{lower}}$ is the lower boundary of the depth increment in mm, $depth_{\text{upper}}$ is the upper boundary of the depth increment in mm, θ_{fc} is the water content at field capacity in vol-%, θ_{wp} is the water content at the permanent wilting point in vol-% and *rocks* denotes the content of rock fragments > 2 mm in vol-%. FAO soil textural classes needed for the PTFs were interpolated from seven German textural classes using log-linear transformation as implemented in the soiltexture::TT.text.transf.X() function in R (Moeys, 2018).

The evaluation of nutrient resources was restricted to three macro-nutrients (nitrogen, phosphorus, sulphur) and one micro-nutrient (copper) – data for other nutrients was unavailable for evaluation. As a simplification, only total elemental concentrations in fine soil (< 2 mm) were considered. Total nitrogen and total sulphur data originated from the database of the German Agricultural Soil Inventory and were obtained via dry combustion using an elemental analyser (LECO TRUMAC, St Joseph, MI, USA). Total phosphorus and total copper were measured in aqua regia extracts (conc. hydrochloric acid / conc. nitric acid 3:1 [v:v]) by inductively coupled plasma optical emission spectroscopy (ICP-OES; Ultima 2, HORIBA Jobin Yvon, Longjumeau, France). Sulphur data was only available for 441 (15 %) of 2931 sites – based on clay and organic C contents this subset did not significantly differ from the global dataset. Phosphorus and copper data was only available for 96 (3 %) of all sites. These 96 sites were core sites of the German Agricultural Soil Inventory, which were representative for German cropland (Gocke et al., subm). Phosphorus and copper data was recorded by M. Gocke (University of Bonn), who shared this data for the scope of the present thesis. Nutrient stock was calculated by multiplying nutrient content with fine soil stock as proposed by Poeplau et al. (2017).

Results. The upper metre of German agricultural soil showed an average capacity to store 142 mm available water (95 % CI, 141 to 143), and contained 10.2 Mg ha^{-1} total nitrogen (95 % CI, 10.0 to 10.3), 8.2 Mg ha^{-1} total phosphorus (95 % CI, 7.1 to 9.8), 1.8 Mg ha^{-1} total sulphur (95 % CI, 1.7 to 1.9), as well as 0.19 Mg ha^{-1} total copper (95 % CI, 0.16 to 0.23; Fig. 6.1). On average, 64 % of the water resource and 40 % (nitrogen) to 68 % (copper) of the nutrients in the upper metre were stored in the subsoil, i.e., in 30–100 cm depth. But, about 20 %(nitrogen, sulphur) to 30 % (water, phosphorus, copper) of all water and nutrient resources stored within the upper metre of German agricultural land were located below RRLs. The previous estimate refers to all resources stored in the upper metre of German agricultural land. But, of course, there was a considerable variability between sites, ranging from almost all resources hidden (RRL at shallow depth) to no hidden resources at sites without RRLs. At compacted sites, on average about 50 % of the water and 30 % to 60 % of the nutrient resources of the upper metre were situated below the uppermost compacted soil layer.

Generally, available water capacity tended to be the highest in loess-derived soil regions (Chernozems of central Germany, also alpine foreland, lower Rhine) and in the upper Rhine plain (Fig. 6.2, Fig. B.4). Soils derived from drift clay along the Baltic Sea showed significantly higher available water capacities than drift sand-derived soils neighbouring to the South (Fig. 6.2, Fig. B.4). In regions with elevated available water capacities (loess, drift clay), the contribution of subsoil to available water capacity of the upper metre was also slightly elevated (Fig. 6.2). In case of total nitrogen stocks, there was a remarkable difference between the East (very low stocks) and West (medium stocks) of northern lowlands, which was mostly explained by differences in subsoil stocks. The amount of nutrient and water resources below RRLs was regionally scattered – only loess derived soil was predominantly without RRLs. In case of sulphur, phosphorus and copper, poor data availability did not allow the evaluation of regional distributions.

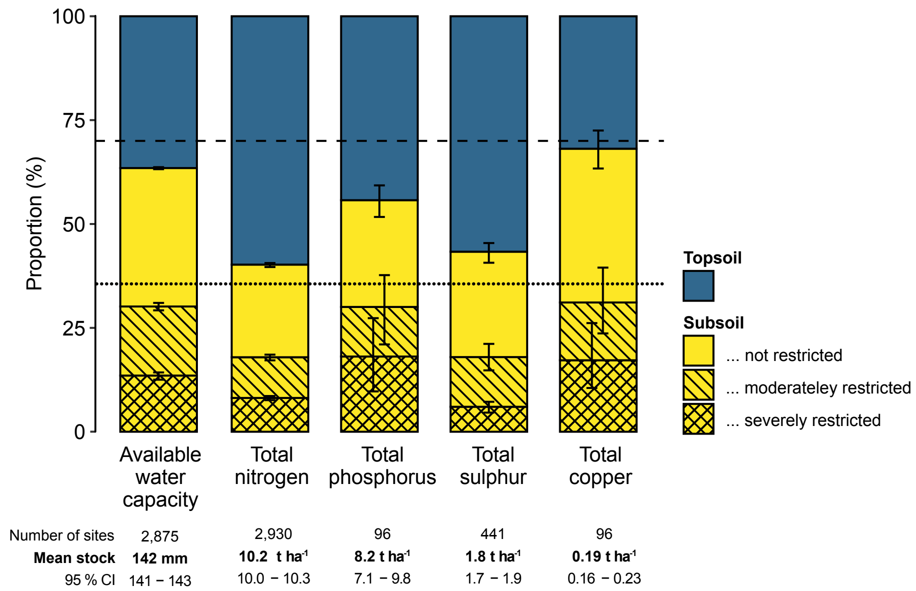


Figure 6.1: Stocks of water and selected nutrient resources in the upper metre of German agricultural soil. Bars show the relative distribution of resources between topsoil (blue, 0–30 cm) and subsoil (yellow, 30–100 cm). Subsoil proportions lower than 70 % (dashed horizontal line) indicate lower resource density in the subsoil than in the topsoil. The dotted horizontal line illustrates the proportion of total organic carbon, which is stored in subsoils. Fill patterns characterise the accessibility of subsoil resources for roots. Error bars illustrate 95 % confidence intervals based on 3000 bootstrapped resamples.

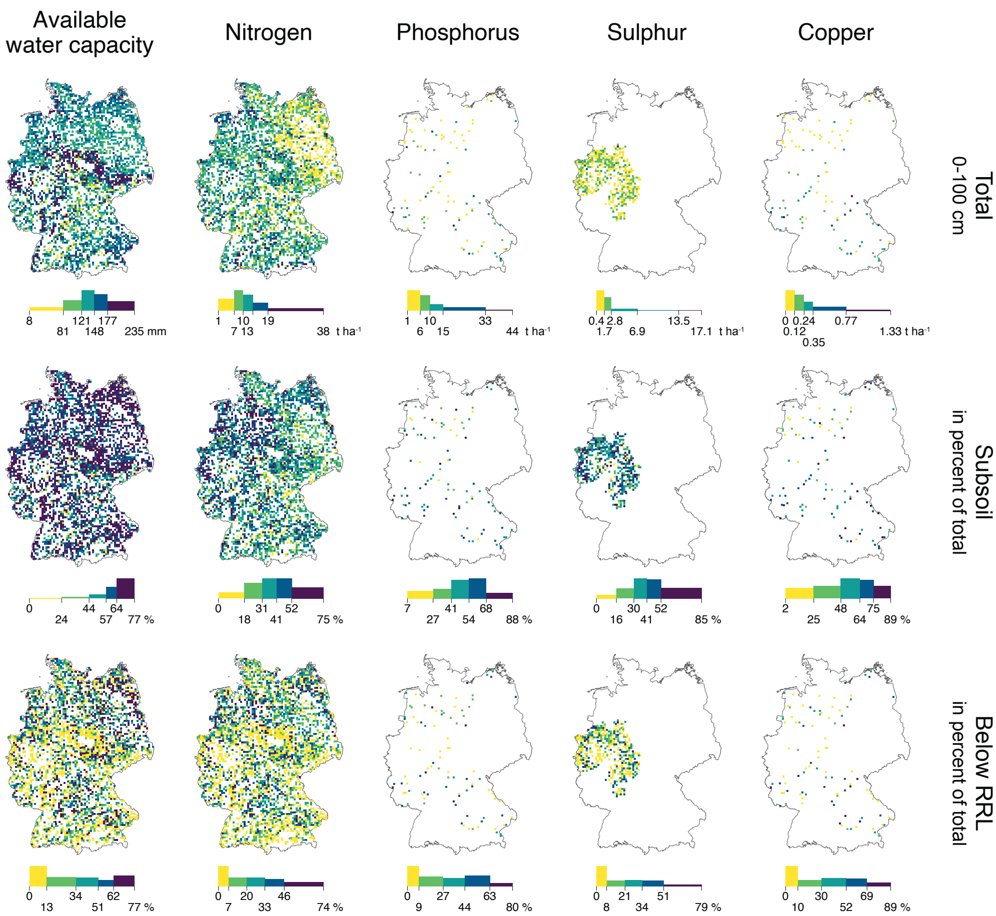


Figure 6.2: Regional distribution of water and selected nutrient resources in German agricultural soils. Top row: total stocks in 0–100 cm depth. Middle row: subsoil stocks in 30–100 cm in percent of total stocks. Bottom row: stocks below root-restricting soil layers (RRL) in percent of total stocks. The classed frequency histogram legends underneath each map show the number of observations in each colour class. Color classes were defined using the Fisher-Jenks algorithm, which aims at minimising the variance within each class while maximising the variance between classes (Fisher, 1958; Jenks & Caspall, 1971).

Discussion. In view of available water capacities being derived with PTFs, which could not be validated with own measurements, and relatively small sample numbers for sulphur, phosphorus as well as copper, the presented results on water and nutrient resources in German agricultural soils should be regarded as rough estimates only. Nonetheless, these resource estimates revealed interesting patterns. The results suggest that the plant-availability of 20 % to 30 % of the water and nutrient resources stored in the upper metre of German agricultural soil is restricted because these resources are situated below RRLs and therefore beyond the easy reach of roots. Especially those resources, whose abundance depended little on organic matter showed large proportions beneath RRLs. Most importantly, this was the case for water. It is estimated that subsoil, i.e., soil in 30–100 cm depth, contributed 64 % to the available water capacity of the upper metre, which indicates that each unit volume of subsoil could retain almost as much water as in topsoil. But the density of organic C was 4.2 times lower in subsoil compared to topsoil (cf. chapter 3). This suggests that organic matter only plays a minor role in determining soil water retention – a view, which concurs with recent paradigm changes concerning the effect of organic matter on soil water storage. Organic matter has long been perceived as key for soil water retention (Hudson, 1994; Rawls et al., 2003). But this view is now increasingly challenged (Minasny & McBratney, 2018; King et al., 2020).
Soil can be regarded as a mediator that stores erratic water input from precipitation to accommodate the continuous water demand of crops. The larger the capacity of soil to store plant-available water, the lower the likelihood of plants experiencing drought stress. RRLs limit the accessibility of soil water resources, making plants more susceptible to drought (chapters 2 and 5). Excluding water resources beneath RRLs, the upper metre of German agricultural soil is capable to store 100 mm of available water. However, the most common crop in Germany, winter wheat, requires about 500 mm per growing season (Roth et al., 2005). The melioration of RRLs could improve the accessibility to additional 42 mm of the available water capacity and, thus, significantly prolong the ability of plants to withstand drought, making yield more stable.

Among the evaluated nutrients, phosphorus and copper showed much larger proportions below RRLs than nitrogen and sulphur. Nitrogen and sulphur are both predominantly organically bound (Amelung et al., 2018), which explains why the proportions of these resources in the subsoil are almost as small as the case for

organic C (Fig. 6.1, dotted line). Phosphorus and copper, however, are more associated with the soil mineral fraction (Amelung et al., 2018) and therefore showed rather similar concentrations throughout the soil profile.
Most agricultural land in Germany is heavily fertilised. Taking the example of the most important nutrient, nitrogen, soils currently receive annually on average 227 kg N ha^{-1} of which 104 kg N ha^{-1} are added as mineral fertiliser and 93 kg N ha^{-1} as organic fertiliser including sewage sludge, manure and biogas digestates (UBA, 2019b). This is about 80 kg ha^{-1} $year^{-1}$ more nitrogen than what is being exported within harvest products and illustrates that yield in a typical German agricultural soil is not limited by nutrient resources. Therefore, I hypothesise that under current fertilisation regimes an improved accessibility of nutrient resources below RRLs would have little effect on yield. In the future, the importance of subsoil nutrients for plant nutrition could increase as the German government aims to reduce excess fertiliser applications (Klages, 2018). Also, phosphorus could be an exception. Bauke et al. (2018) recently observed increasing phosphorus uptake from subsoil with increasing levels of topsoil fertilisation in field experiments. However, the extent to which enhanced phosphorus uptake from subsoil could increase yield on farms at high levels of topsoil fertilisation remains to be tested.

Considering that 20 % to 30 % of the water and nutrient resources are hidden below RRLs, the melioration of RRLs could significantly improve plant nutrition. Under current fertilisation practices (most land is fertilised in excess) and irrigation practices (only 3 % of cropland is irrigated), I hypothesise that German food and fibre production would benefit especially from the enhanced access to subsoil water. Meliorating RRLs would allow plants to better exploit water resources from the soil and significantly improve the resilience of German agricultural land against drought – an ecosystem property which will likely gain even further importance in future (Samaniego et al., 2018).

6.2.2 Melioration measures to facilitate resource uptake from subsoil

The BonaRes project $Soil^3$, funded by the German Federal Ministry of Education and Research (BMBF) under the "National Research Strategy BioEconomy 2030", currently aims at developing management strategies for improving water and nutrient uptake from subsoils. In the project, four different subsoil melioration strategies are examined to achieve this goal: deep ploughing, deep loosening, a novel approach of deep slotting, and biodrilling (Frelih-Larsen et al., 2018). Deep ploughing, deep loosening and deep slotting are mechanical methods of soil melioration while biodrilling is a biological melioration method (chapter 4). The concepts of deep ploughing and deep loosening, the latter sometimes being also referred to as subsoiling, have been introduced in chapter 5 of this thesis (Fig. 5.1). The novel deep slotting method has been designed within the Soil^3 project. In principle, it builds on earlier work by Bradford & Blanchar (1980) and Jayawardane et al. (1995) in that it involves mixing of subsoil with saw dust, chopped straw or other organic material along slots (trenches) that are several metres apart. However, the Soil^3 approach of deep slotting is novel in that a new slotting device has been engineered, optimised to minimise topsoil deterioration when incorporating the organic material into the subsoil (Jakobs et al., 2017; Frelih-Larsen et al., 2018; Jakobs et al., 2019). The fourth option for subsoil management discussed within Soil^3 is biodrilling. Biodrilling involves the cultivation of pioneer plants with particularly deep and thick roots, which form continuous macropores (biopores) into the subsoil that can serve subsequent crops as "highways" into the subsoil (Kautz, 2015). For Germany, most research on biodrilling has been done so far using alfalfa (*Medicago sativa* L.) as the pioneer plant (e.g., Gaiser et al., 2012; Kautz & Köpke, 2010).

All melioration methods have to be adapted to local site conditions in order to be successful. Otherwise melioration can fail and even decrease the productivity, trafficability and workability of sites (cf. chapter 5). A leading German expert on subsoil melioration in the second half of the twentieth century noted (Müller, 1985):

nur meliorationsbedürftige Böden
und meliorationsfähige Böden
sind meliorationwürdig.

Roughly translated, this means that not every soil needs to be meliorated and not every soil is capable of being meliorated. Only those soils that are in need and are capable of melioration should also be meliorated (Fig. 6.3). In the following, I will attempt to apply this guideline from the past to identify promising target regions for improved subsoil management on German agricultural land in the future. As a model scenario, I will address the melioration of compacted soil

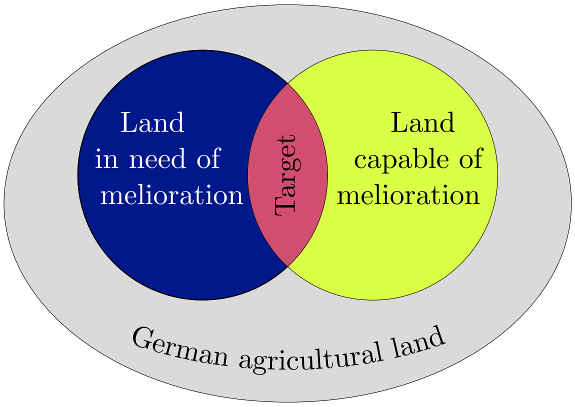


Figure 6.3: Strategy to identify target sites for subsoil melioration.

by means of deep ploughing, deep loosening, deep slotting with the new Soil[3] technique and biodrilling with alfalfa. I focus specifically on the melioration of compacted soil because in chapter 2 high compactness has been identified as the dominant soil-borne cause for restricted root growth, i.e., resource uptake, in German agricultural soils (cf. chapter 2).

Land in need of melioration: "meliorationsbedürftige Böden"

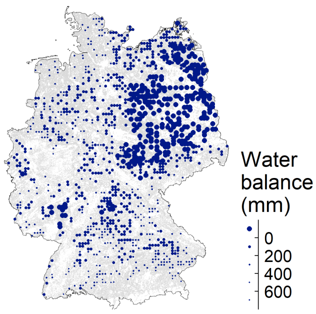
Fertile soil, which supports high yield and high yield stability shows little potential for further improvement. Therefore, efforts on improving the accessibility of subsoil resources should focus on poor agricultural land where the elongation of deep roots is severely restricted. Based on an evaluation of the German Agricultural Soil Inventory, high compactness is by far the most prevalent soil property that hinders plant roots from accessing subsoil resources on German agricultural land (chapter 2). Sustainable melioration of compacted soil profiles (i) would significantly improve access to about 50 % of the total available water capacity of the upper metre, and (ii) could increase the amount of nutrient resources within the reach of plant roots, by up to 40 % for total nitrogen and 100 % for total phosphorus[4]. The meta-analysis about the effect of deep tillage on crop yield suggests that crops in dry areas would benefit most from the improved access to plant-available water (chapter 5). In terms of economic return of subsoil melioration, I hypothesise that cropland would benefit more from subsoil melioration than grassland. In spring, annual crops tend to demand much more resources from the soil than grassland (Wendland et al., 2014). Also, anthropogenic compaction was

[4]Estimates based on data presented in the previous section

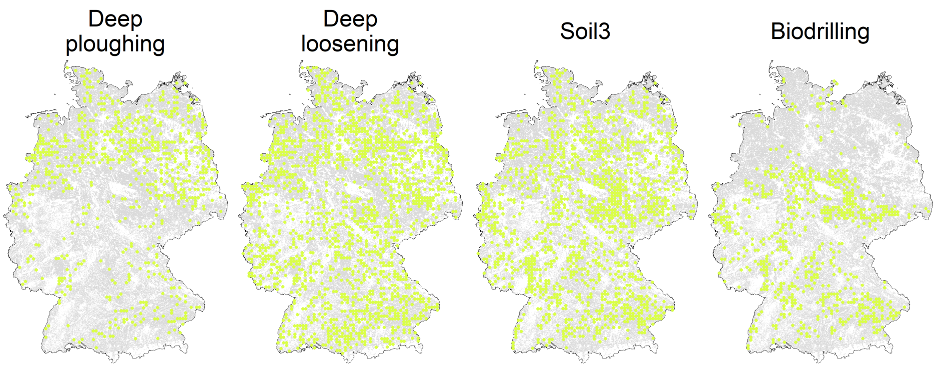
much more severe in cropland soil compared to that in grassland soil (chapter 2). In conclusion, I attribute compacted croplands in relatively dry areas the highest need for subsoil melioration. Compacted cropland is regionally highly scattered in Germany (Fig. 2.3). But with respect to drought stress, there is a pronounced gradient: drought stress tends to increase from west to east with only minor exceptions like in viticultural areas along the Main river and upper Rhine valley (DWD, 2019a). Thus, in east Germany, compacted cropland shows an increased need for melioration (Fig. 6.4a).

Land capable of being meliorated: "meliorationsfähige Böden"

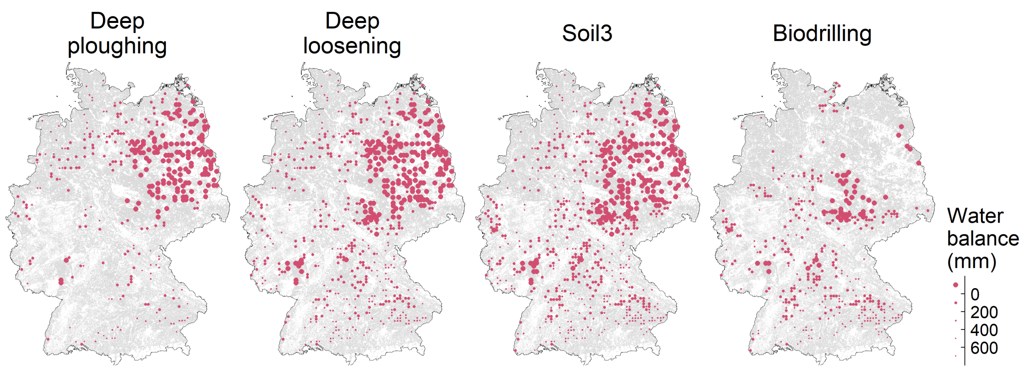
Depending on the method, there are different exclusion criteria for subsoil melioration (Table 6.1, Fig. 6.5). These criteria comprise conditions under which conducting the melioration measure is either not possible at all, or accompanied with a high risk of causing negative side effects. An obvious example are shallow soils, like Leptosols of the Swabian Jura. By definition, these soils show only a small subsoil volume and therefore are not capable of being meliorated. Another example are organic soils. In the present scenario, organic soils are not relevant for melioration because they typically show no compacted soil layers (chapter 2). However, the chosen melioration technologies could also hardly be applied in organic soil because alfalfa is not a suitable crop to be grown in organic soil (Hartmann et al., 2014) and mechanical soil meliorations would conflict with the contemporary protection status of organic soils (Zeitz, 2014). The remaining exclusion criteria only affect specific melioration methods (Table 6.1). Drain pipes represent an exclusion criteria for mechanical melioration measures because the latter could damage the pipes. But the presence of drain pipes does not interfere with biodrilling. Sites with shallow groundwater can only be meliorated by deep ploughing and deep loosening if they developed from sand – as in many Gleyic Podzols of the Weser-Ems area, where deep ploughing used to be very popular (chapter 4). But heavy soil with shallow groundwater is hard to be meliorated by deep ploughing or deep loosening because moist clay would smear instead of shatter (chapter 5). Furthermore, groundwater could cause organic material incorporated via the Soil^3 method to decompose anaerobically and trigger significant emissions of nitrous oxide and other greenhouse gases (Weier et al., 1993). Alfalfa performs very poor on sites with shallow groundwater (Hartmann et al., 2014). Furthermore, alfalfa is also not a suitable crop for acid soil, very sandy soil, and soil with large rock frag-



(a) Compacted cropland sites in need of melioration. Point size increases with decreasing mean annual water balance (DWD, 2019a), which serves as an indicator for drought stress – the lower the water balance, the more drought stress, the larger the need of melioration.



(b) Sites where melioration technology could theoretically be applied best with low likelihood of causing negative side effects.



(c) Target sites for melioration.

Figure 6.4: Regional distribution of sites in need of melioration (top), sites capable of being meliorated (middle) and target sites that both need and can be meliorated (bottom). Points show affected sites from the 8 x 8 km sampling grid of the German Agricultural Soil Inventory. Grey background shows the total spatial extent of German agricultural land (BKG, 2020).

ment content (chapter 4). Large rock fragment and large clay contents represent barriers for adopting deep ploughing. Rock fragment content typically increases with increasing depth (Jacobs et al., 2018), and deep ploughing would increase the rock fragment content of topsoil because deep ploughing turns the soil profile. In soil with large clay content, such as Vertisols and Vertic Cambisols, deep ploughing has never gained high popularity because it lifted big chunks of clay to the surface soil (chapter 5, Scheffer & Meyer, 1970). Both rocks and large chunks of clay hinder the use of agricultural machinery for seeding and harvest (Kreitmayr & Demmel, 2014). In soil with $> 70\,\%$ silt content, deep ploughing and deep loosening may cause the complete collapse of soil structure and further compaction instead of loosening (chapter 5). Permanent grassland allows only deep loosening for soil melioration (Schulte-Karring, 1995). All other melioration methods would cause significant damage of the grass sod, which could conflict with the protection status of permanent grassland (Möckel, 2016a) and farmers could loose subsidy payments (Möckel, 2016b).

In order to judge the overall capability of sites to be meliorated, I simplified the exclusion criteria described above and projected each of them to a binary scale (1=criterium applies; 0=criterium does not apply). For this, I defined threshold values, which are shown in Table 6.1. If at least one of the exclusion criteria applied to a given site and melioration method, the site was regarded as incapable of being meliorated with the respective method. The disadvantage of this approach was that most threshold values were arbitrary and might vary within a certain range, which would change the results for individual sites. However, regional patterns were quite robust towards minor changes of the threshold values (results not shown). The advantage of the applied simplified, binary approach was that it was transparent, it judged each site based on exactly the same criteria, and the results are reproducible.

Overall, the exclusion criteria defined above eliminated 76 % of the sampling sites of the German Agricultural Soil Inventory for deep ploughing, 48 % for deep loosening, 54 % for the Soil^3 method and 77 % for biodrilling (Table 6.1, Fig. 6.5). The regional distribution of the remaining sites, which were theoretically capable of melioration, differed depending on the melioration technology (Fig. 6.4b). Deep loosening and the Soil^3 method showed the largest potential area of application. Sites suitable for deep loosening occurred everywhere in Germany, except large parts of the loess areas and in drift clay soils along the coast of the Baltic Sea, where drainage pipes were the dominant exclusion criteria for deep loosening (Fig. 6.5).

Table 6.1: Exclusion criteria for conducting deep ploughing (DP), deep loosening (DL), the novel Soil^3 method (Soil^3) and/or biodrilling (BP).

Property	Definition used in this study	Affected technology
Shallow soil	Non-diggable, solid bedrock in < 1 m depth	All
Rock fragments	> 20 vol-% rock fragments† (> 2 mm)	DP,BP
Clay	Main texture class: clay†*	DP
Silt	> 70 % silt†	DP,DL
Sand	Main texture class: sand†*	BP
Acidity	$pH_{H_2O} < 5^{\dagger}$	BP
Drain pipes	Subsoil with drainage pipes	DP,DL,Soil^3
Groundwater	Pedogenic horizon code "r"†*	DP$^{\circ}$,DL$^{\circ}$,Soil^3,BP
Grassland	Continuous grassland use for ≥ 5 years	DP,Soil^3,BP
Organic soil	> 7.82 % soil organic C†*	All

† at least one depth increment per site
* according to AD-HOC-AG Boden (2005)
$^{\circ}$ only in heavy soil

In case of the Soil^3 method, the potential area of application excluded large parts of southern Germany and along the North Sea (both grassland dominated) and it excluded many sites in the Weser-Ems area (many hydromorphic soils). Deep ploughing and biodrilling both showed relatively small potential areas of application. In case of deep ploughing, the majority of suitable sites were located in the northern lowlands on soils that developed from drift sand (Fig. B.4). Potential areas for applying biodrilling were mainly confined to soil derived from loess in central Germany, lower Rhine river and south of the Danube river.

Target sites for melioration: "meliorationswürdige Böden"

Considering both the need and capability of soil to be meliorated, I propose compacted cropland in east Germany as the most promising target for mechanical subsoil melioration (Fig. 6.4c). I propose east Germany because of (i) lower water balances (higher drought stress) than elsewhere in Germany, and (ii) the widespread distribution of drift sand-derived soil, which shows little pedological constraints for mechanical soil profile modifications. In other regions of Germany, compacted cropland (i) tended to show a lower need to be meliorated, and/or (ii) a lower capability to be meliorated mechanically. My suggestion to focus mechanical melioration efforts on compacted, sandy soil in east Germany is corroborated by historic field experiments. Mechanical soil profile modifications conducted by Rauhe & Müller (1959) and Rauhe (1960) on sandy soil at the Leibniz Centre for Agri-

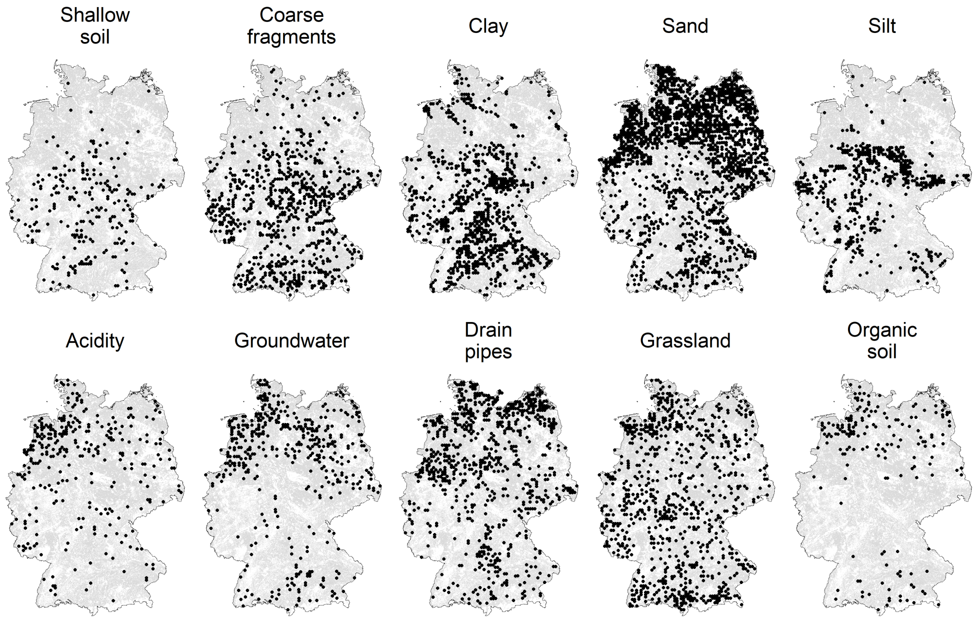


Figure 6.5: Regional distribution of exclusion criteria for some subsoil melioration technologies as detailed in Table 6.1. Black dots show affected sites from the German Agricultural Soil Inventory. Grey background shows the full spatial extent of agricultural land in Germany (BKG, 2020).

cultural Landscape Research (ZALF) in Müncheberg have produced some of the most positive crop yield responses documented in Germany (chapter 5). Egerszegi (1959) showed deep soil profile modifications in sandy soil to be particularly successful, if organic material was incorporated into the subsoil. This attributes high potential to applying the novel Soil^3 method in sandy soil of east Germany. But as this method is quite new it requires further testing – there could be exclusion criteria for the Soil^3 method, which are not known yet.

The proposed target area for biodrilling is smaller than for mechanical melioration options (Fig. 6.4c). This can be mainly attributed to the relatively narrow ecological niche of the chosen model species used for biodrilling (alfalfa). Considering both need and capability of melioration, I attribute biodrilling with alfalfa the highest potential in loess-derived, compacted soil, especially in relatively dry areas such as in the southern and eastern periphery of the Harz mountains. Biodrilling with alfalfa might also be a promising technique to meliorate the mostly pedogenically compacted heavy clay soils such as Vertisols and Vertic Cambisols, which are frequently encountered in Franconia and in the north eastern part of

Baden-Württemberg. Other plants, which are capable of forming large continuous biopores like chicory (*Cichorium intybus* L.) could extend the potential area of application for biodrilling (Han et al., 2015a), but this still needs to be better tested.

Subsoil melioration in Germany – next steps

The target regions proposed above point to regions where, from a pedological and technological point of view, adopting melioration technology could be the most beneficial. Within target regions, there is an increased likelihood of encountering agricultural land, which is both in need and capable of melioration. Vice versa, outside target regions, this likelihood is lower. Thus, target regions inform about regional trends. However, at the field scale, the need and capability of sites to be meliorated can vary considerably. Neighbouring fields, of which only one is compacted or with drainage pipes, can be encountered in every region. Because of this heterogeneity, it is important to inspect every site individually before conducting a melioration measure. The criteria listed in Table 6.1 could provide a rough guide for such field inspections. Compacted, sandy sites and compacted loess-derived sites seem to represent promising targets for mechanical and biological melioration, respectively. However, before promoting these measures to farmers, further data is needed, especially with respect to the performance and exclusion criteria of the novel Soil^3 method and biodrilling. Finally, in order to actually implement subsoil melioration in practice, socio-economic aspects have to be considered. For example, even if applying the Soil^3 method on compacted cropland could double yield, the melioration would still gain little popularity if the machinery and needed compost material was not available. Planting alfalfa could find little acceptance among farmers because they would need to take their cropland out of the normal production cycle for at least one, better two growing seasons (Frelih-Larsen et al., 2018). Barriers hindering the practical implementation of subsoil melioration are identified best in close dialogue with farmers, farmer unions and with stakeholders of melioration technology. Such dialogues will be key to successfully implement subsoil melioration in practice.

Frelih-Larsen et al. (2018) raised the concern that high costs could deter many farmers from adopting subsoil melioration technology. This points to the urgent need for a detailed cost-benefit analysis of subsoil melioration. Considering recent price increases for agricultural land, I hypothesise that the profitability of subsoil melioration could improve in future. Since 2007, the average hectare prize of German agricultural land has risen 2.8-fold from 9205 € to 25 485 € (Destatis, 2020a). On the one hand, the increased prize of agricultural land can be explained by its decreased availability – in the past 20 years, almost one million hectares of German agricultural land has been lost (World Bank, 2020), mostly because of soil sealing in the periphery of urban areas (Gardi et al., 2015). At the same time, the demand for farmland has been increasing, supported by subsidies for bioenergy production and an increasing number of non-agricultural investors (Tietz, 2018). Rising prices reflect the increasing scarcity of agricultural land in Germany. In the absence of more usable soil area, subsoil melioration could give way to more usable soil volume (Kuntze, 1982), increasing the productivity, yield stability and thus economic benefit of meliorated sites. Interestingly, the highest price increase for agricultural land occurred in east Germany, which is also the proposed target area for mechanical subsoil melioration. Since 2007, the hectare price for agricultural land has risen 4.3-fold in Mecklenburg-Vorpommern and 3.6-fold in Brandenburg (Destatis, 2020b). The results of this thesis suggest, that in large parts of these federals states, investments in more soil volume via subsoil melioration could provide a viable alternative to investments in more soil area.

6.3 Conclusions

More than half of German agricultural land exhibits severe barriers for root penetration. This limits crop yield because plants cannot tap the full potential of the water and nutrient resources offered by subsoils. High compactness represents the dominant soil-borne cause for restricted rooting. Most compacted soil layers are of pedogenic origin. However, the present thesis provides strong evidence for trafficking soil with heavy farm machinery to have significantly increased the spatial extent of compacted soil in Germany. Future agricultural management should intensify existing efforts to prevent the further spread of anthropogenic soil compaction. Once established, compacted soil layers and other soil-borne causes for restricted root growth are difficult to meliorate – meliorations are laborious, costly and have to be adapted to site specific conditions. Nonetheless, the melioration of RRLs deserves greater attention. For one, it is climate-smart and the sustainable loosening of compacted soil could result in a significant increase of subsoil C stocks. The greatest potential of meliorating RRLs, however, lies in its ability to unlock additional deep nutrient and, especially, water resources to plants. Easily accessible, plant-available water reserves from subsoils are key to making rainfed agro-ecosystems more resilient against drought. In meliorating RRLs, German food and fibre production could become better prepared for a future, which will be shaped by climatic change.

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Appendix A

▷ Chapter 2

Table A.1: Variables used to predict soil compactness, i.e., packing density.

Name	Type*	Explanation	Source**
Climate			
Temperature	C	Multi-annual monthly averaged daily minimum air temperature in 2 m height [°C]	DWD_Temp.min
Soil climate	F(22)	Soil-climate regions	Roßberg, D. et al. (2007)
NDVI	C	Multi-annual mean normalized difference vegetation index in June	Gebbert, S. (unpublished)
Precipitation	C	Multi-annual mean of precipitation [mm year^{-1}]	DWD_Precip.mean
Sunshine	C	Multi-annual mean of sunshine duration [hours year^{-1}]	DWD_Sun
Geology			
Geomorphology	F(10)	Geomorphological terrain classes	BGR_GMK1000
Slope	C	Slope in degrees	BKG_DGM25
Soil parent rock	F(11)	Soil parent rock	BGR_BAG5000
Soil region	F(11)	Bodengroßlandschaft (engl. large soil landscape)	BGR_BÜK200
Stratigraphy	F(6)	Stratigraphic units based on AD-HOC-AG Boden (2005)	GASI_Field
Management & socio-economy			
Canola, beet and legumes	C	Share of rape seed, sugar beet and legumes in crop rotation [-]	GASI_Farmer
Drainage	F(2)	Drainage (yes/no)	GASI_Field
Farm size	C	Total farm size [ha]	GASI_Farmer
Field size	C	Field size [ha]	GASI_Farmer
Historical land-use	C	Number of years since current land-use [years]	GASI_Farmer
Land-use	F(3)	Annual crops, perennial crops or grassland. For predicting compactness by land-use, this parameter was neglected.	GASI_Farmer, GASI_Field
Maize	C	Share of maize in crop rotation [-]	GASI_Farmer
Soil			
Biopores	C	Biopore density [vol-%]	GASI_Field
Clay	C	Clay content [mass-% of fine soil <2mm]	GASI_Lab
Depth	C	Sampling depth [cm]. For predicting the compactness by depth increment, this parameter was neglected.	GASI_Field
Groundwater	F(8)	Depth to groundwater table. Levels according to AD-HOC-AG Boden (2005).	GASI_Field
Illuviated clay	C	Area percentage of soil horizon with clay illuviation	GASI_Field
Oximorphic features	C	Area percentage of oximorphic features at profile wall	GASI_Field
pH	C	pH measured in deionized water (1:5)	GASI_Lab
Reducing soil horizon	C	Area percentage of soil horizon with reducing conditions in > 300 days per year (pedogenic horizon symbol "r")	GASI_Field
Reductimorphic features	C	Area percentage of reductimorphic features at profile wall	GASI_Field
Rock fragments	C	Rock fragments [vol-%]	GASI_Lab
Sand	C	Sand content [mass-% of fine soil < 2 mm]	GASI_Lab
SOC	C	Total organic carbon [mass-% of fine soil < 2 mm]	GASI_Lab
Soil type	F(10)	Soil type modified after AD-HOC-AG Boden (2005)	GASI_Field
Stagnogleyic horizon	C	Area percentage with stagnogleyic soil horizon	GASI_Field
TIC	C	Total inorganic carbon [mass-% of fine soil < 2 mm]	GASI_Lab

* C = continuous variable; F(L) = categorical variable with L levels

**

BGR_BAG5000	Bundesanstalt für Geowissenschaften und Rohstoffe: BAG5000 V3.0, Hannover, 2007
BGR_BÜK200	Bundesanstalt für Geowissenschaften und Rohstoffe: BÜK200, Hannover, 2018
BGR_GMK1000	Bundesanstalt für Geowissenschaften und Rohstoffe: GMK1000R V2.0, Hannover, 2006
BKG_DGM25	Bundesamt für Kartographie und Geodäsie: Digitales Geländemodel Gitterweite 25 m (http://www.bkg.bund.de), 2018
DWD_Precip.mean	DWD Climate Data Centre (CDC): Multi-annual grids of precipitation height over Germany 1981-2010, v1.0, 2017
DWD_Sun	DWD Climate Data Center (CDC): Multi-annual grids of annual sunshine duration over Germany 1981-2010, v1.0, 2017
DWD_Temp.min	DWD Climate Data Center (CDC): Multi-annual grids of monthly averaged daily minimum air temperature
GASI_Farmer	German Agricultural Soil Inventory: Farmer questionnaire
GASI_Field	German Agricultural Soil Inventory: Soil profile descriptions by field workers
GASI_Lab	German Agricultural Soil Inventory: Laboratory
Gebbert, S. (unpublished)	Derived from Landsat (NASA, USGS) images
Roßberg, D. et al. (2007)	Roßberg, D., Michel, V., Graf, R., Neukampf, R., 2007. Definition von Boden-Klima-Räumen für die Bundesrepublik Deutschland. Nachrichtenblatt des deutschen Pflanzenschutzdienstes 59, 155-161.

Table A.2: Conversion of root count classes to continuous scale.

Root count classes based on AD-HOC-AG Boden (2005)		Present study
Category	Range	Value
[-]	Root count dm^{-2}	
W0	0	0.0
W1	1-2	1.5
W2	3-5	4.0
W3	6-10	8.0
W4	11-20	15.0
W5	21-50	35.0
W6	> 50	50.0

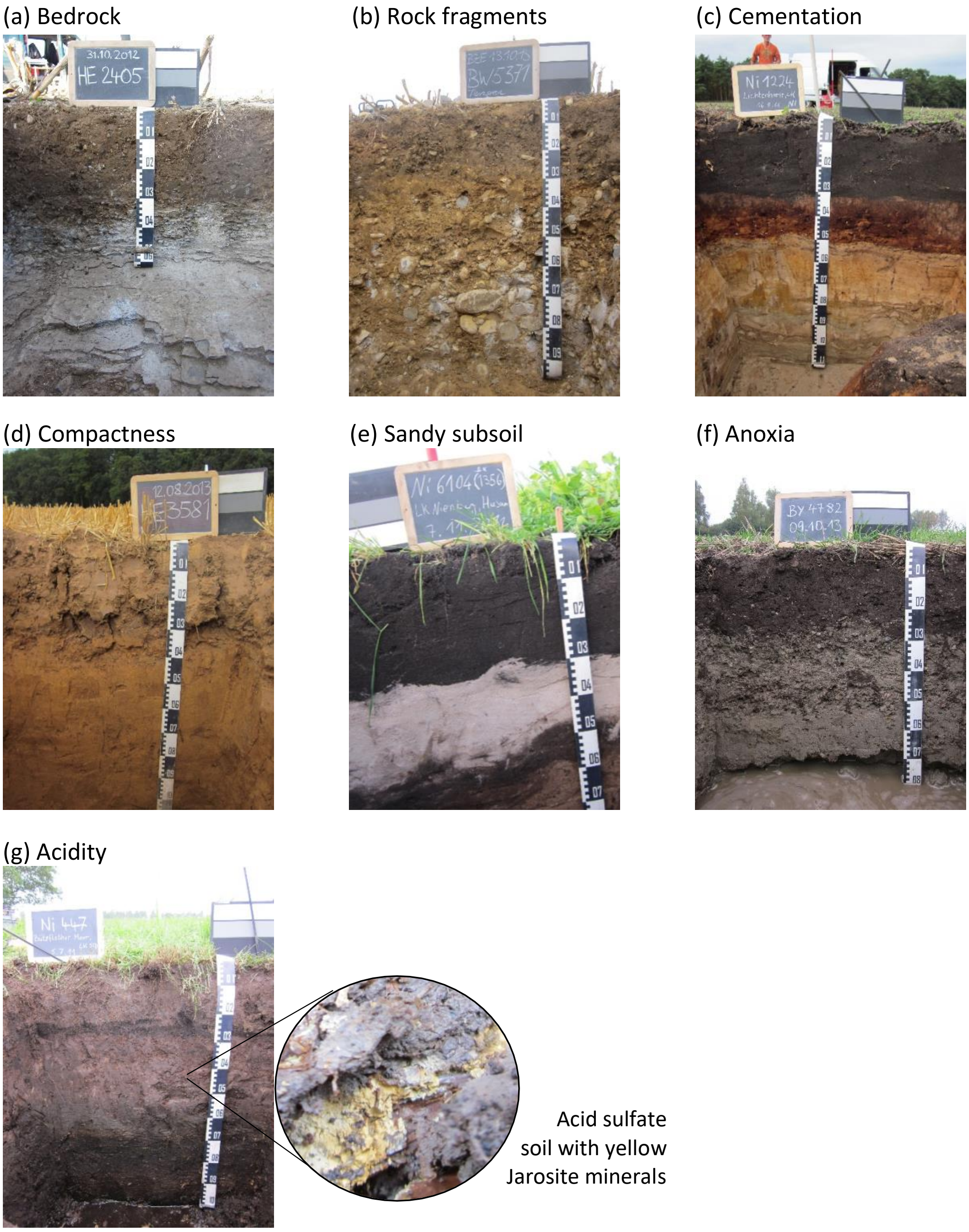


Figure A.1: Examples of soil profiles with root-restricting layers.

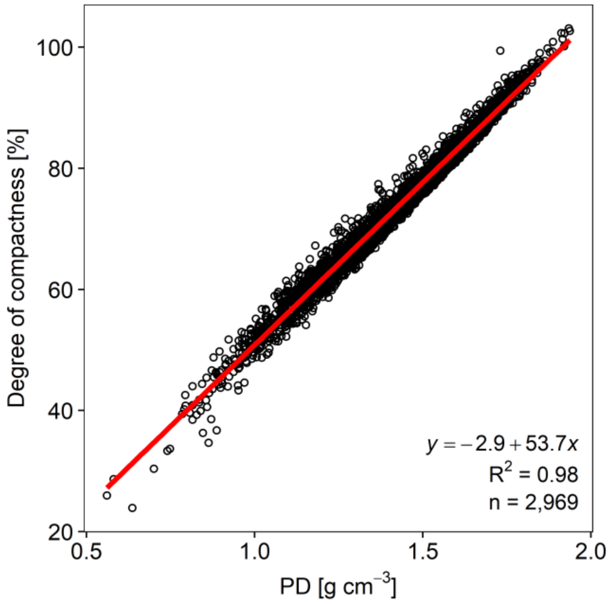


Figure A.2: Degree of soil compactness as a function of packing density (PD). Degree of compactness was calculated after Naderi-Boldaji & Keller (2016). Plot is shown for all soil samples in the German Agricultural Soil Inventory with similar characteristics, as in Naderi-Boldaji & Keller (2016): 4 % < sand content < 57 %; 16 % < clay content < 60 %; 1 % < SOC < 8.7 %.

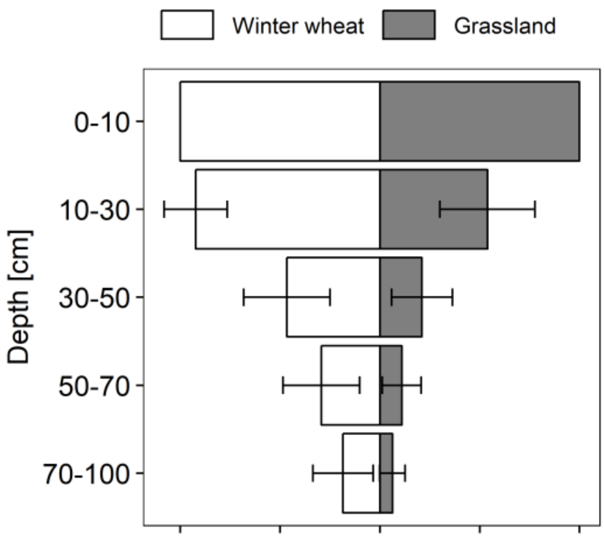


Figure A.3: Mean relative root counts (root count in 0–10 cm divided by root count in depth i) of winter wheat and grassland by depth. Error bars represent standard deviations.

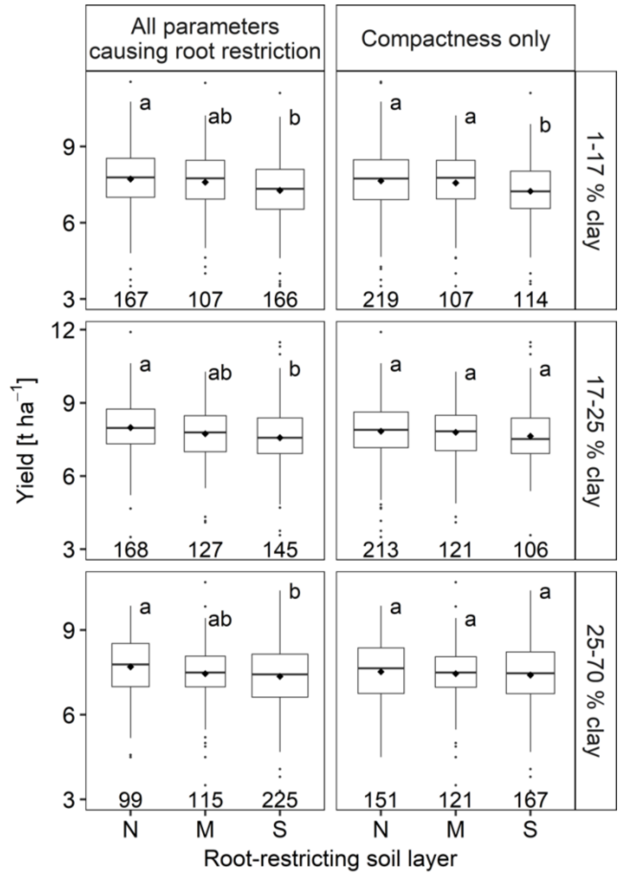


Figure A.4: Boxplot of grain yield for winter wheat grown on sites with no (N), with moderate (M) and with severe (S) root restrictions stratified by average soil clay content in 0–100 cm depth. Yields sharing the same letter are not significantly different at $p < 0.05$ level. Boxplot width is proportional to the observation number.

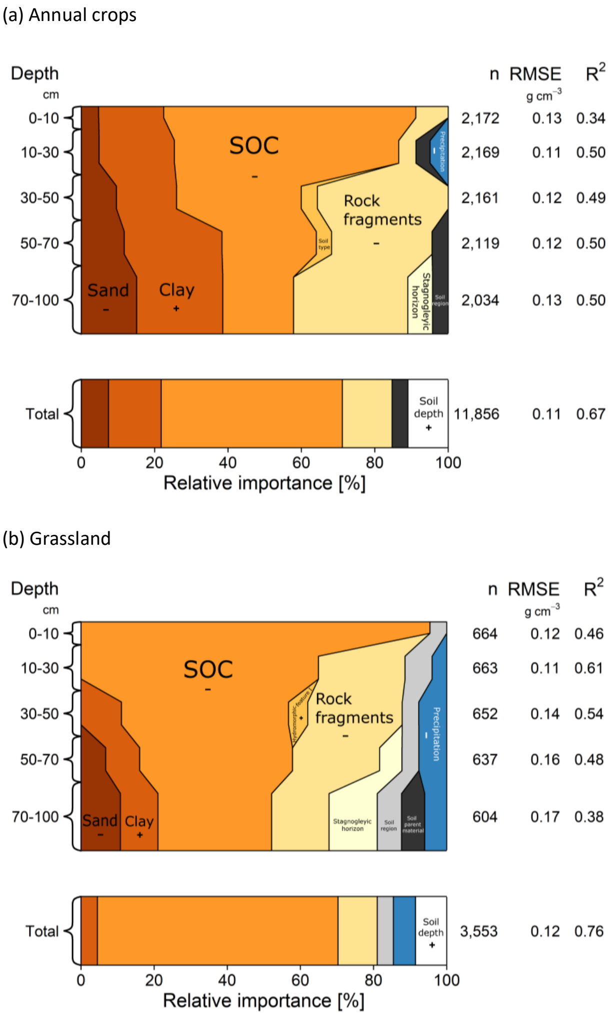


Figure A.5: Significant predictors of the packing density of mineral soils under crops (a) and grassland (b) by depth. Brown and yellow colours represent pedology, grey represents geology and geomorphology, green represents land use and blue represents climate-related variables. Areas are proportional to the relative importance of the predictors. Each model is characterised by the number of observations in the training data ("n") and errors from out-of-bag data (root mean square error ("RMSE") and R-squared ("R^2"). Positive marginal effects of continuous predictors on packing density are illustrated as "+" and negative effects as "-".

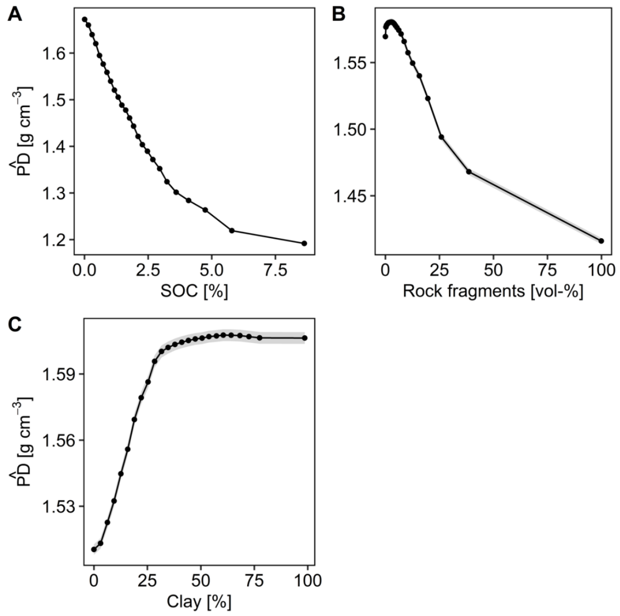


Figure A.6: Partial dependence of the top four predictors of packing density ($\widehat{PD}$) in the Random Forest model, which included all land uses and depths (as illustrated in Fig. 2.7).

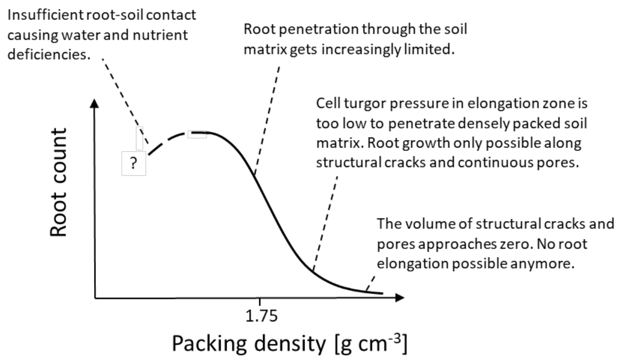


Figure A.7: Theoretical effect of packing density on root counts in structured soil.

Appendix B

▷ Chapter 3

B.1 Spectral modelling of POC:TOC ratios

Using the training data shown in Fig. AB.1, spectral modelling was performed as follows. Predictions were made for all combinations of the following pre-treatments, models and associated hyperparameters: (i) pre-treatments: Savitzky-Golay transformation with differentiation order 1, polynomial order 2 and window size 3 (yes/no); standard normal variate transformation (yes/no); and (ii) models: partial least squares (pls) regression (number of components: from 2 to 40 in steps of 4); ranger (mtry: 15, 30, 60, 120, 240, 480, 720 or 960; min.node.size: 1, 10 or 20; splitrule: variance, extratrees or maxstat); cubist (committees: 1, 10, 50 or 100; neighbours: 0, 3 or 9). The following approaches were also tested: (i) prediction of square-root transformed POC and MOC contents independently and correction of the predicted POC and MOC values by TOC recovery, (ii) log-ratio transformation of POC and MOC contents following Aitchison (1982) and Jaconi et al. (2019a), (iii) prediction of POC:TOC and MOC:TOC ratios independently and correction of the predicted ratios based on 100 % constraint, and (iv) log-ratio transformation of POC:TOC and MOC:TOC ratios. Model performances were evaluated based on the ratio of performance to deviation (RPD) metric, calculated as the standard deviation of the reference values divided by the root mean square error from leave-one-site-out validation. RPD values above 2.0 are indicative of good predictions (Chang & Laird, 2002). Based on RPD, the top ten parameter combinations were selected, plus the best parameter combination for each model type (pls, cubist, ranger) and each modelling approach (log-ratio transformation of POC and MOC content vs. log-ratio transformation of POC:TOC and POC:MOC; prediction of POC and MOC contents vs. prediction of POC:TOC and MOC:TOC ratios). Tests were then conducted on whether averaging the results of any of these models would outperform the best single model. The best ensemble consisted of the following three models: (1) Savitzky-Golay + standard normal variate transformations, ranger (mtry=120, min.node.size=10, splitrule=maxstat), log-ratio transformation of POC and MOC; (2) standard normal variate transformation, pls (ncomp=14), predicting POC:TOC and MOC:TOC ratios separately and correcting the predicted ratios based on 100 % constraint; (3) cubist (committees=10, neighbours=0), log-ratio transformation of POC:TOC and MOC:TOC ratios. This ensemble resulted in an RPD value of 2.46 (Fig. AB.2) and was used to predict the POC:TOC ratio of all unseen soil samples.

B.2 Data collection for machine learning

For machine learning, only explanatory variables were used that were indicative of processes governing soil organic C dynamics at regional scale. The following processes/drivers were considered:

- recent C input: C input data calculated by Jacobs et al. (subm); proportion of C_4 plants (maize) in crop rotation etc.
- historic C input: characterisation of soil parent material etc.
- translocation of C within soil profiles: soil reference groups, soil horizon symbols etc.
- soil transport (erosion/deposition): slope, relief, soil horizon symbols etc.
- stabilisation/turnover: texture, Gr-horizons, redoximorphic features.

Furthermore, we included climate-related covariates because climate is a major soil-forming factor and can have various effects on C input and C stabilisation. In order to describe climate, for each site included in the German Agricultural Soil Inventory its value was extracted with respect to the following indicators:

Since many of these indicators were highly correlated, a principal component analysis (PCA) was performed and only the top-loading indicators were included as covariates in the models. Principal components (PCs) were accepted if they exhibited eigenvalues greater than Kaiser's criterion of 1.00. Retained PCs were rotated orthogonally following the varimax method to enhance interpretability. The PCA yielded four PCs that, combined, explained 92 % of the total variance:

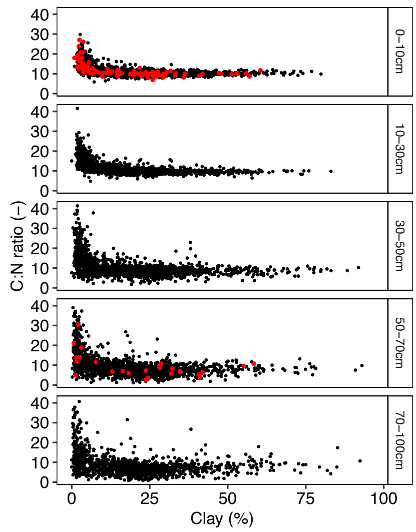


Figure B.1: Calibration samples (red) used for spectral modelling of POC:TOC ratios in unseen soil samples (black).

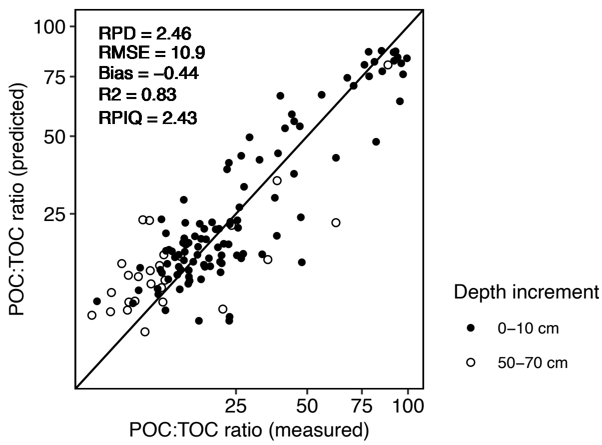
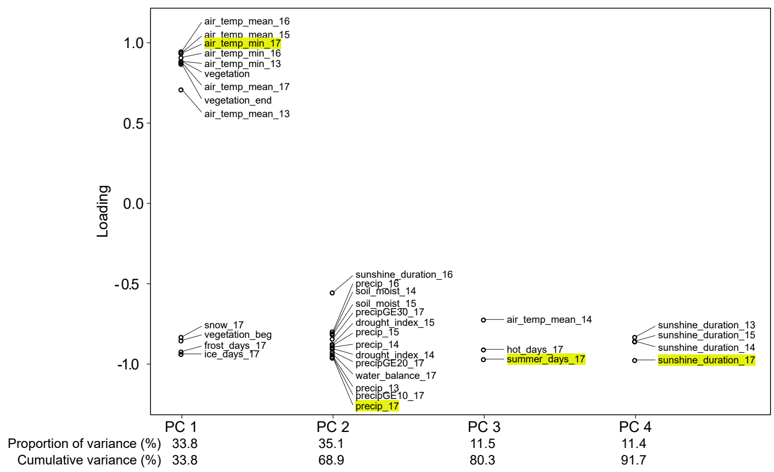


Figure B.2: Relationship between measured (reference) and predicted particulate organic carbon (POC) in the percentage of total organic carbon (TOC) content based on near-infrared spectra. The solid line represents the 1:1 line.

Name	Description	Time period	Source
air_temp_mean_13 air_temp_mean_14 air_temp_mean_15 air_temp_mean_16 air_temp_mean_17	Monthly averaged mean daily air temperature in 2 m height above ground (°C)	1981-2010 (Jan-Mar) 1981-2010 (Apr-Jun) 1981-2010 (Jul-Sep) 1981-2010 (Oct-Dec) 1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Grids of the multi-annual mean temperature (2m) over Germany 1981-2010, version v1.0
air_temp_min_13 air_temp_min_16 air_temp_min_17	Mean of the monthly averaged minimum daily air temperature in 2 m height above ground (°C)	1981-2010 (Jan-Mar) 1981-2010 (Oct-Dec) 1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Grids of the multi-annual minimum temperature (2m) over Germany 1981-2010, version v1.0
drought_index_14 drought_index_15	Drought index after de Martonne (mm/°C)	1981-2010 (Apr-Jun) 1981-2010 (Jul-Sep)	DWD Climate Data Centre (CDC): Multi-annual grids of drought index (de Martonne) over Germany 1981-2010, version v1.0
frost_days_17	Number of frost days. Definition of frost day: minimum air temperature < 0 °C	1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of frost days over Germany 1981-2010, version v1.0
hot_days_17	Number of hot days. Definition of hot day: maximum air temperature >= 30 °C	1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of hot days over Germany 1981-2010, version v1.0
ice_days_17	Number of ice days. Definition of ice day: maximum air temperature < 0 °C	1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of ice days over Germany 1981-2010, version v1.0
precip_13 precip_14 precip_15 precip_16 precip_17	Multi-annual mean of precipitation (mm)	1981-2010 (Jan-Mar) 1981-2010 (Apr-Jun) 1981-2010 (Jul-Sep) 1981-2010 (Oct-Dec) 1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of precipitation height over Germany 1981-2010, version v1.0
precipGE10_17	Number of days with precipitation >= 10 mm	1961-1990 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of days with precipitation >= 10 mm over Germany 1961-1990, version v1.0
precipGE20_17	Number of days with precipitation >= 20 mm	1961-1990 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of days with precipitation >= 20 mm over Germany 1961-1990, version v1.0
precipGE30_17	Number of days with precipitation >= 30 mm	1961-1990 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of days with precipitation >= 30 mm over Germany 1961-1990, version v1.0
snow_17	Number of days with snow cover. Definition of snow cover: snow depth >= 1 cm at morning reading (nowadays 7 UTC)	1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of days with snowcover over Germany 1981-2010, version v1.0
soil_moist_14 soil_moist_15	Soil moisture at 5 cm depth in percent of total plant available soil water. Assumptions: Constant wilting point (13 vol-%) and field capacity (37 vol-%)	1991-2010 (Apr-Jun) 1991-2010 (Jul-Sep)	DWD Climate Data Centre (CDC): Multi-annual grids of soil moisture in 5 cm depth under grass and sandy-loam 1991-2010
summer_days_17	Number of summer days. Definition of summer day: maximum air temperature >= 25 °C	1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of number of summer days over Germany 1981-2010, version v1.0
sunshine_duration_13 sunshine_duration_14 sunshine_duration_15 sunshine_duration_16 sunshine_duration_17	Multi-annual mean of sunshine duration in hours	1981-2010 (Jan-Mar) 1981-2010 (Apr-Jun) 1981-2010 (Jul-Sep) 1981-2010 (Oct-Dec) 1981-2010 (Jan-Dec)	DWD Climate Data Centre (CDC): Multi-annual grids of sunshine duration over Germany 1981-2010, version v1.0
vegetation_beg	First flowering of *Forsythia* (mean day of the year)	1992-2015	DWD Climate Data Centre (CDC): Multi-annual grids of the beginning of the vegetation period in Germany 1992-2015
vegetation_end	First leaf fall of *Quercus robur* (mean day of the year)	1992-2015	DWD Climate Data Centre (CDC): Multi-annual grids of the end of the vegetation period in Germany 1992-2015
vegetation	Mean duration of growing season (vegetation_end - vegetation_beginning)	1992-2015	
water_balance_17	Multi-annual water balance	1971-2000	DWD Climate Data Centre (CDC): Multi-annual grids of water balance over Germany 1971-2000

PC 1 clustered variables with reference to temperature and the length of the growing season, PC 2 was related to precipitation and water balance, PC 3 indicated hot (summer) days, and PC 4 was related to sunshine duration. For all subsequent analyses, we used the following climate variables:

Table AA.1 provides an overview of all 39 variables used to predict the depth distribution of TOC content, C:N and TOC:POC ratios, and $\delta^{13}C$ and $\delta^{15}N$ values.



PC	Name	Nice name used in the present study
1	air_temp_min_17	Temperature
2	precip_17	Precipitation
3	summer_days_17	Summer days
4	sunshine_duration_17	Sunshine

Table B.1: Variables used to predict organic C proxies.

Name	Type*	Explanation	Source**
Climate			
Pedo-climatic zone	F(15)	Pedo-climatic zones modified after Rossberg, D. et al. (2007). Translated factor levels (original): Central Uplands (Schwarzwald, Bayrischer Wald, Erzgebirge, Thueringer Wald, Rhoen, Harz, Teutoburger Wald, Sauerland, Briloner Höhen, osthessische Mittelgebirgslagen, Odenwald, Spessart, Hocheifel, Hunsrück, Westerwald, Mittellagen in Rheinland-Pfalz/Saarland, Verwietterungsböden in den Höhenlagen (Bayern), Ost-Westfalen, Lippe, Harrstrang, Bergisches Land); Diluvial soil (sandige diluviale Böden des nordostdeutschen Binnentieflandes, trocken-warme diluviale Böden des ostdeutschen Tieflandes, diluviale Böden der Altmark und Überlappung nördliches Niedersachsen); Alpine Foreland (Tertiär-Hügelland Donau-Süd, Gäu, Donau- und Inntal, Moräne-Hügelland und Alpenvorland); Baltic Sea (mittlere diluviale Böden MV und Uckermark, NW-Mecklenburg und Küstengebiet; vorpommersche Sandböden; schleswig-holsteinisches Hügelland); Baltic Sea (Schwäbische Alb, Baar, Albflächen, Ostbayrisches Hügelland, oberes Gäu und körnermaisfähige Übergangslagen); Ems-Weser-Geest (Geest, nordwestliches Weser-Ems-Gebiet, Elbe-Weser-Dreieck); Central loess plain (Lössböden der Ackerebene); Rhine plain (Rheinebene und Nebentäler); Loess periphery (Lössböden in den Übergangslagen); Regolith periphery (Verwitterungsböden in den Übergangslagen); Lüneburg Heath (Lüneburger Heide); SW of Weser-Ems (Weser-Ems Südwest); Börde (Jülicher Börde, zentralhessische Ackerbaugebiete, Warburger Börde); North Sea (Niedersächsische Küsten- und Elbmarsch, Marsch (Nord)); Other (Hochrhein-Bodensee, mittleres Niedersachsen, oberer Mittelrhein, Nordwestbayern-Franken, Alpen, Südhannover, Oderbruch).	Rossberg, D. et al. (2007)
Precipitation	C	Multi-annual mean of precipitation (mm year^{-1})	DWD_Precip.mean
Summer days	C	Number of summer days	DWD_Sommer
Sunshine	C	Multi-annual mean of sunshine duration (hours year^{-1})	DWD_Sun
Temperature	C	Multi-annual monthly averaged daily minimum air temperature in 2 m height (°C)	DWD_Temp.min
Geology			
Age of parent material	C	Age of the soil parent material (Ma)	BGR_Guek250
Chronostratigraphy	F(3)	Chronostratigraphic units. Holocene, Pleistocene or older.	GASI_Field
Curvature1	F(3)	Vertical surface curvature based on AD-HOC-AG Boden (2005), Feld 13. None, convex or concave.	GASI_Field
Curvature2	F(3)	Horizontal surface curvature based on AD-HOC-AG Boden (2005), Feld 13. None, convex or concave.	GASI_Field
Elevation	C	Elevation above sea level (m)	BKG_DGM25
Geomorphology	F(10)	Geomorphological terrain classes. Translated factor levels (original): Depression, wet (Tiefenbereich mit mittlerer bis sehr hoher Bodenfeuchte); Depression, dry (Tiefenbereich mit sehr geringer bis geringer Bodenfeuchte); Lowland, wet (sehr gering bis gering geneigter Unterhang im Norddeutschen Tiefenland); lowland, dry (mittel geneigter Mittel- oder Oberhang im Norddeutschen Tiefenland); flat (gering bis mäßig geneigter Unterhang im Alpenvorland); Alpine Foreland, steep (mäßig geneigter Mittel- oder Oberhang im Alpenvorland); Upland, flat (sehr gering bis gering geneigter Hang im Bergland); Upland, steep (mäßig bis stark geneigter Hang im Bergland); Culmination1 (sehr gering bis gering geneigter Oberhang im Bergland); Culmination2 (Scheitelbereich in den Hochlagen der Mittelgebirge).	BGR_GMK1000
Lithogeny	F(8)	Environmental conditions during lithogeny ("Genese"): fluvio-limnetic (fluvial oder limnisch); glacial (glaziär); sedimentary (sedimentär); marine (marin); igneous-metamorphic (magmatisch oder metamorph); palustrine (ombrogen oder topogen); fluvio-marine (brackisch); volcanic (vulkanisch).	BGR_Guek250
Parent material	F(14)	Soil parent material. Factor levels (original German name): Tidal deposit (Sedimente im Gezeitenbereich); Overbank deposit (Auensedimente); Bench gravel (Terrassen- und Schotterablagerungen); Drift sand (Sande und mächtige sandige Dechschichten); Drift clay and shallow drift sands (Geschiebemergel-/lehme im Wechsel mit geringmächtigen Deckschichten); Drift clay (Geschiebemergel/-lehme); Loess (Loesse und Loessderivate); Sandy loess (Sandloesse); Carbonate rock (Caronatgesteine; Kalk- und Mergelgesteine); Pelitic rock (Tongesteine i.w.S.); Psammite (Sandsteine); Mafic igneous rock (Basische Magmatite und Metamorphite); Acid igneous rock (Saure Magmatite und Metamorphite); Peat (Hoch- und Niedermoortorfe).	BGR_BAG5000
Petrology	F(9)	Petrology ("Petrographie"): pelitic (pelitisch); psammitic (psammitisch); sedimentary (sedimentär); clastic (klastisch); metamorphic (Anchimetamorphit, Impakt..., Meta...); psephitic (psephitisch); organic (pflanzlich); volcanic (pyroklastisches, Tephra, vulkanklastisches, Vulkanit, Mikromagmatit); plutonic (Tektonit).	BGR_Guek250
Slope	C	Slope in degrees	BKG_DGM25
Soil region	F(11)	Soil regions (Bodenregionen). Factor levels (original German name): Kuestenholozaen (Coastal alluvium); Riverine plain (Ueberregionale Flusslandschaften); Young Drift (Jungmoränenlandschaften); Old Drift (Altmoränenlandschaften); Alpine Foreland (Deckenschotterplatten und Tertiärhügelländer im Alpenvorland); Loess plain (Loess- und Sandloesslandschaften); Central Uplands 1 (Berg- und Huegellaender mit hohem Anteil an nichtmetamorphen carbonatischen Sedimentgesteinen); Central Uplands 2 (Berg- und Huegellaender mit hohem Anteil an Ton- und Schluffschiefern); Central Uplands 3 (Berg- und Huegellaender mit hohem Anteil an Magmatiten und Metamorphiten); Central Uplands 4 (Berg- und Huegellaender mit hohem Anteil an nichtmetamorphen Sedimentgesteinen im Wechsel mit Loess); Central Uplands 5 (Berg- und Huegellaender mit hohem Anteil an nichtmetamorphen Sand-/Schluff-/Ton- und Mergelgesteinen)	BGR_BÜK200
Terrain	F(4)	Topographical relief based on AD-HOC-AG Boden (2005), Feld 14. Factor levels (German code): Slope (H); Depression (T); Erosion surface (V); Culmination (K).	GASI_Field
Management			
C input: fertiliser	C	Mean C input from organic fertilizer (t ha^{-1} year-^{1})	Jacobs, A. et al. (submitted)
C input: roots	C	Mean C input from roots and rhizodeposits (below ground) (t ha^{-1} year^{-1})	Jacobs, A. et al. (submitted)
C input: total	C	Mean Total C input from above and below ground (t ha^{-1} year-^{1})	Jacobs, A. et al. (submitted)
Canola, beet and legumes	C	Share of canola (Brassica napus), beet (mostly Beta vulgaris) and legumes (mostly Trifolium sp.) in crop rotation (-)	GASI_Farmer
Land use	F(3)	Annual crops, perennial crops or grassland	GASI_Farmer, GASI_Field
Livestock	C	Livestock units (=Großvieheinheiten) per hectare. One livestock unit represents 500 kg, i.e. roughly the weight of one bull.	GASI_Farmer
Maize	C	Share of maize in the crop rotation of the past 10 years (%)	GASI_Farmer
N input: fertiliser	C	Mean N input from fertilizers (t ha^{-1} year-^{1})	Jacobs, A. et al. (submitted)
Soil transport	F(3)	No soil transportation, soil accumulation (deposition) or abrasion (removal of earth) based on AD-HOC-AG Boden (2005), Feld 18.	GASI_Field
Soil			
Biopores	C	Biopore density (vol-%) as described in Schneider & Don (2019)	GASI_Field
Clay	C	Clay content (%)	GASI_Lab
Gr-horizon	C	Area percentage of soil horizon with reducing conditions in > 300 days per year (pedogenic horizon symbol "r" as defined by AD-HOC-AG Boden (2005))	GASI_Field
Groundwater	F(5)	Mean depth to groundwater table. Levels according to AD-HOC-AG Boden (2005), Feld 53, "mittlerer Grundwasserstand".	GASI_Field
Oximorphic features	C	Area percentage of oximorphic features at profile wall based on AD-HOC-AG Boden (2005), Feld 30	GASI_Field
pH	C	pH measured in deionized water (1:5)	GASI_Lab
Reductimorphic features	C	Area percentage of redoximorphic features at profile wall based on AD-HOC-AG Boden (2005), Feld 31	GASI_Field
Relic topsoil	C	Fossile or relic A, O, L or H-Horizon based on AD-HOC-AG Boden (2005)	GASI_Field
Rock fragments	C	Rock fragment content (vol-%)	GASI_Lab
Sand	C	Sand content (%)	GASI_Lab
Soil group	F(11)	WRB Reference Soil Group	GASI_Field
Soil horizon	F(12)	Master soil horizon symbol (Horizonthauptsymbol) based on AD-HOC-AG Boden (2005). Factor levels (English translation based on Wittmann et al. 1997): A (mineral topsoil horizon; epipedon); B (mineral subsoil horizon characterized by a change of colour and mineral composition of the parent material resulting from the accumulation of topsoil constituents, which were removed from the overlying horizon or/and weathering in situ; contains less than 75 vol-% of residual parent rock and no lithogenic carbonate (primary carbonate) in the fine-earth fraction); C (unaltered or unweathered material similar to parent material); E (plaggen-horizon; humus content similar to Ah-horizon); G (horizon affected by groundwater, which causes the development of redoximorphic features); H (organic horizon originating from residue of peat-forming plants); M (horizon of fluvial, colluvial soils from translocated soil-material, humus content like Ah); P (subsoil horizon on claystone or clay (>45 % clay) with prismatic to subangular blocky structure and temporarily wide cracks (> 1 cm in 50 cm depth)); R (man made horizon by deep cultivation (>40cm), humus content like Ah); S (subsoil horizon affected by a perched watertable; surface water stagnation characterized by certain redoximorphic features (mottles, concretions, bleaching) or permanently inadequate aeration); T (subsoil horizon from the solution residue of carbonate rock, clay content >65 %, <5% carbonate, bright brown. Yellow to brownish red colour and distinct angular blocky structure (T from terra)).	GASI_Field
TIC	C	Total inorganic carbon (g kg^{-1})	GASI_Lab

* C = continuous variable; F(L) = categorical variable with L levels

**

BGR_BAG5000	Bundesanstalt für Geowissenschaften und Rohstoffe: BAG5000 V3.0, Hannover, 2007
BGR_BÜK200	Bundesanstalt für Geowissenschaften und Rohstoffe: BÜK200, Hannover, 2018
BGR_GMK1000	Bundesanstalt für Geowissenschaften und Rohstoffe: GMK1000R V2.0, Hannover, 2006
BGR_Guek250	Bundesanstalt für Geowissenschaften und Rohstoffe: GUEK250 V1.2, Hannover, 2010
BKG_DGM25	Bundesamt für Kartographie und Geodäsie: Digitales Geländemodel Gitterweite 25 m (http://www.bkg.bund.de), 2018
DWD_Precip.mean	DWD Climate Data Centre (CDC): Multi-annual grids of precipitation height over Germany 1981-2010, v1.0, 2017
DWD_Sommer	DWD Climate Data Centre (CDC): Multi-annual grids of annual sunshine duration over Germany 1981-2010, v1.0, 2017
DWD_Sun	DWD Climate Data Centre (CDC): Multi-annual grids of annual sunshine duration over Germany 1981-2010, v1.0, 2017
DWD_Temp.min	DWD Climate Data Centre (CDC): Multi-annual grids of monthly averaged daily minimum air temperature
GASI_Farmer	German Agricultural Soil Inventory: Farmer questionnaire
GASI_Field	German Agricultural Soil Inventory: Soil profile descriptions by field workers
GASI_Lab	German Agricultural Soil Inventory: Laboratory
Jacobs, A. et al. (submitted)	Jacobs A, Poeplau C, Weiser C, Fahrion-Nitschke A, Don A (submitted) Exports and inputs of organic carbon on agricultural soils in Germany. Nutrient Cycling in Agroecosystems.
Roßberg, D. et al. (2007)	Roßberg, D., Michel, V., Graf, R., Neukampf, R., 2007. Definition von Boden-Klima-Räumen für die Bundesrepublik Deutschland. Nachrichtenblatt des deutschen Pflanzenschutzdienstes 59, 155-161.

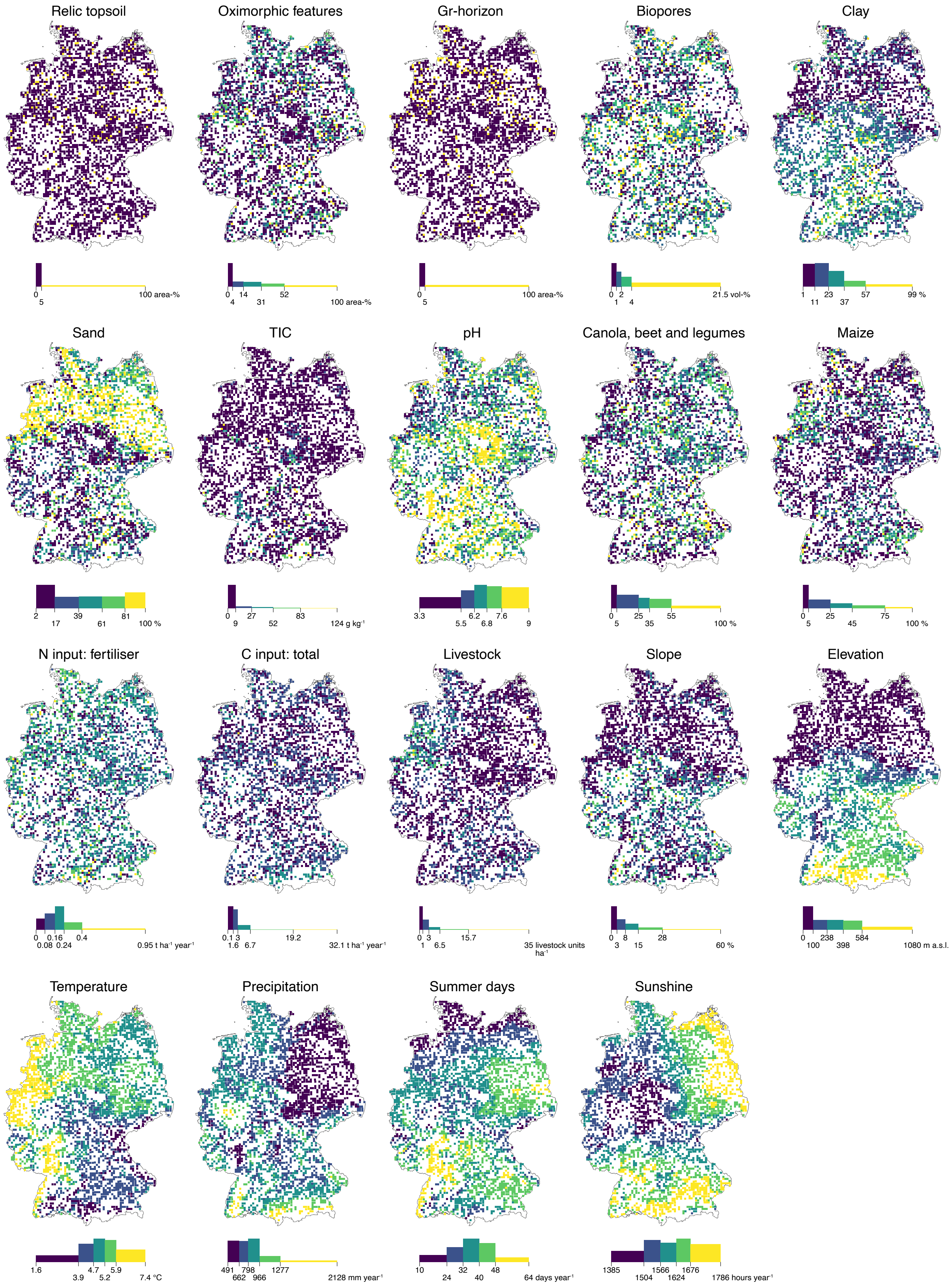


Figure B.3: Maps of important continuous predictors for organic C proxies. For variables that vary with respect to latitude/longitude but also with soil depth, the 50–70 cm depth increment is shown.

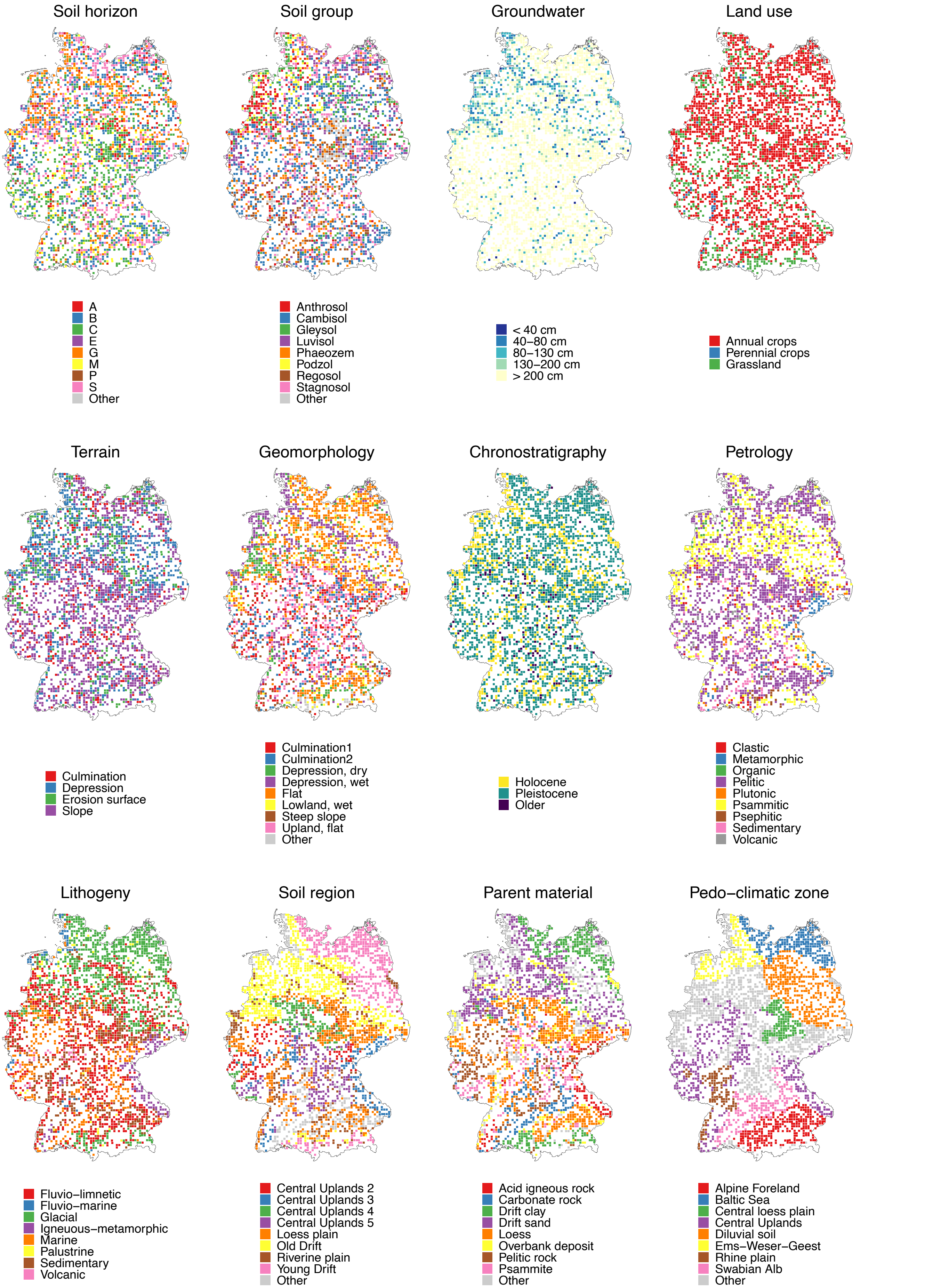


Figure B.4: Maps of important categorical predictors for organic C proxies. For variables that vary not only with respect to latitude/longitude but also with soil depth (soil horizon and chronostratigraphy), the 50–70 cm depth increment is shown.

B.3 More figures

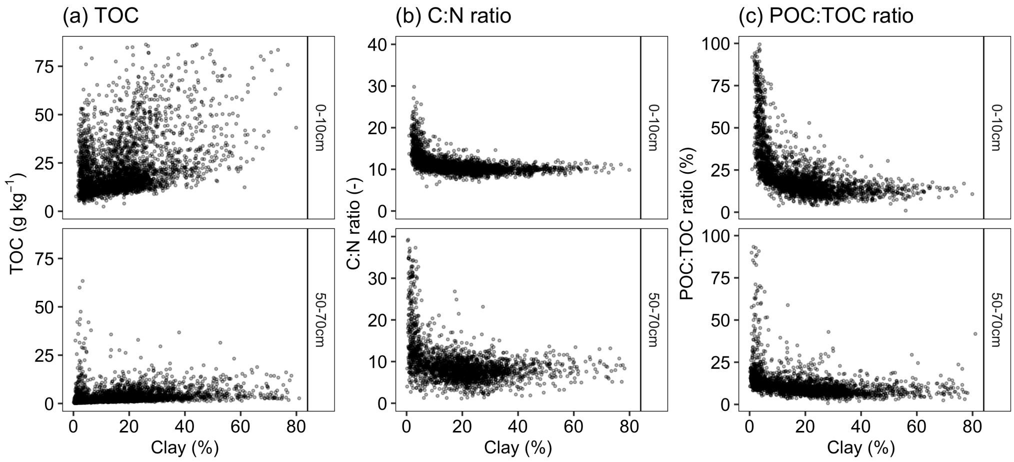


Figure B.5: TOC, C:N ratio and POC:TOC ratio vs. clay content in 0–10 cm depth (top row) and 0–70 cm depth (bottom row).

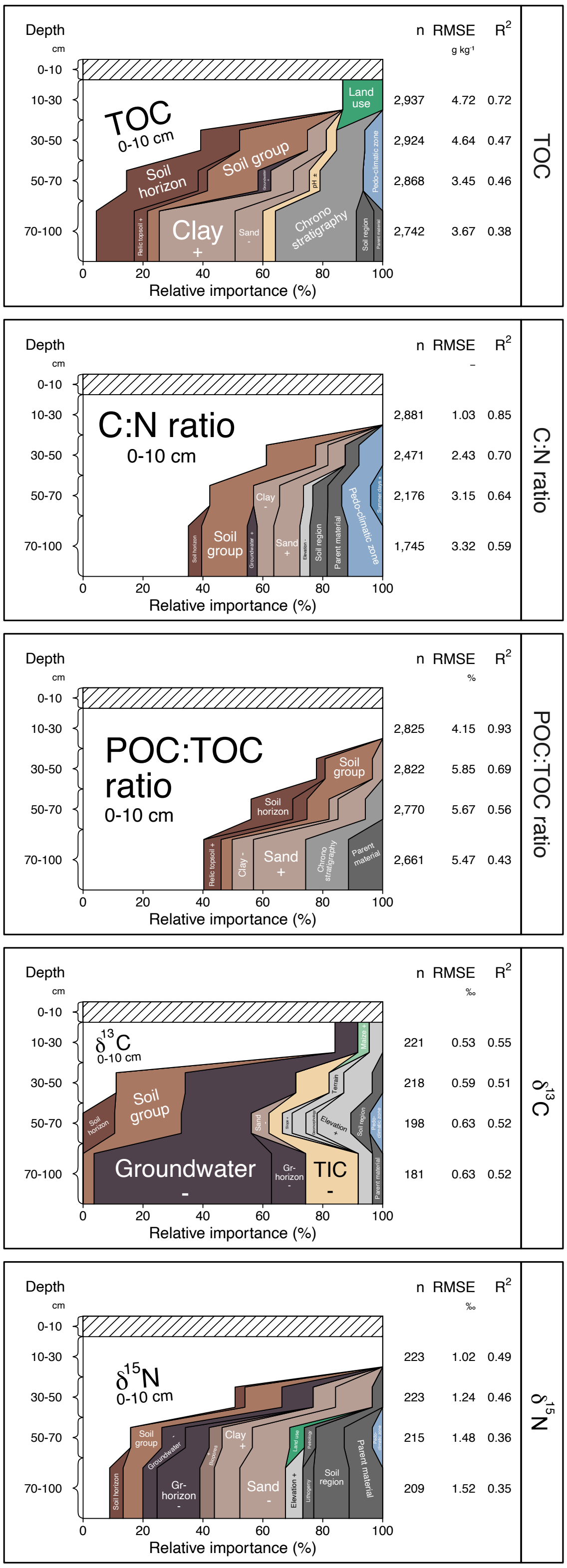


Figure B.6: Important predictors of TOC content, C:N and POC:TOC ratios, as well as $\delta^{13}C$ and $\delta^{15}N$ values by depth. Results for predicting bulk soil values with information from uppermost sampling layer at 0–10 cm depth.

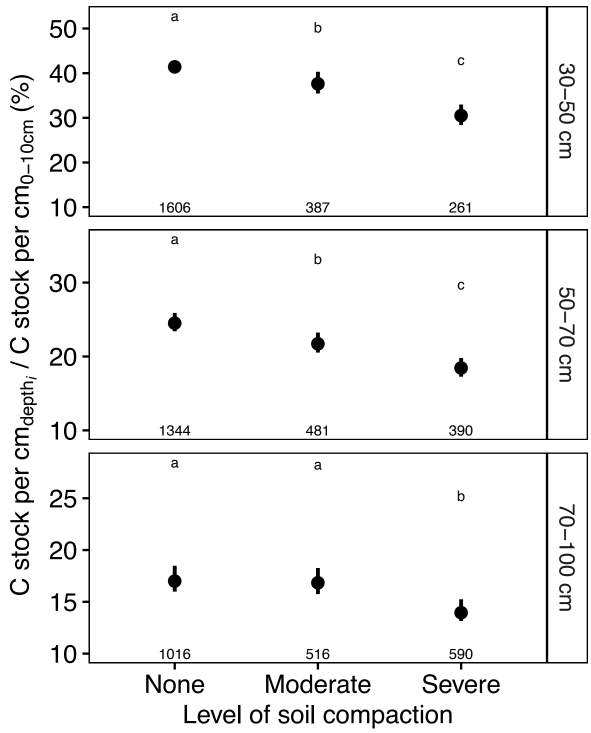


Figure B.7: Depth gradients of C stocks in cropland soil without compaction, moderate compaction and severe compaction. Mean values are shown with error bars representing bootstrapped 95 % confidence intervals. Different letters indicate significant differences at the 5 % level.

Appendix C

▷ Chapter 4

C.1 How biopore abundance was measured

In the field, biopore abundance was recorded for each soil horizon and in ordinal ranks. This was done visually by trained experts who only used the field charts below as a guide (Fig. C.1). No other tool was used.
Individual abundance estimates were made depending on biopore origin (not specified, earthworm burrow or taproot), current occupancy status (not specified, abandoned or inhabited) and biopore diameter (not specified, small, medium or large). Evaluating the data at this level was not possible because (i) subcategories remained often unspecified, and (ii) observation numbers were too low to show significant differences at this level. Therefore, all biopore types were aggregated and evaluated together. Aggregation required the conversion of ordinal classes to continuous scale. This conversion was done by (i) assigning each ordinal abundance class (e.g., f1) its respective interval at continuous scale (e.g., 1 to < 2 vol-%) according to the field charts, and (ii) calculating the average of the minimum and maximum values for each interval (Table reftabA31). Finally, individual abundance estimates were summed up to yield total biopore abundance for each soil horizon.

Table C.1: Overview of the dataset used to explain observed soil melioration measures.

Name	Type*	Explanation	Source**
Climate			
Temperature	C	Multi-annual monthly averaged daily minimum air temperature in 2 m height [°C]	DWD_Temp.min
Soil climate	F(22)	Soil-climate regions	Roßberg, D. et al. (2007)
NDVI	C	Multi-annual mean normalized difference vegetation index in June	Gebbert, S. (unpublished)
Precipitation	C	Multi-annual mean of precipitation [mm year^{-1}]	DWD_Precip.mean
Sunshine	C	Multi-annual mean of sunshine duration [hours year^{-1}]	DWD_Sun
Geology			
Soil parent material	F(11)	Groups of soil parent material	BGR_BAG5000
Soil region	F(11)	Soil region	BGR_BÜK200
Geomorphology	F(10)	Geomorphological terrain classes	BGR_GMK1000
Terrain	F(4)	Topographical relief	GASI_Field
Curvature1	F(3)	Horizontal surface curvature	GASI_Field
Curvature2	F(3)	Vertical surface curvature	GASI_Field
Slope	C	Slope in degrees	BKG_DGM25
Organic soil	F(2)	Organic soil? Yes or no	Jacobs, A. et al. (2018)
Geography			
Administrative region	F(16)	Federal states (NUTS-1 regions)	BKG_NUTS
Longitude	C	Easting (UTM 32)	GASI_Field
Latitude	C	Northing (UTM 32)	GASI_Field
Management & socio-economy			
Drainage	F(2)	Field drained? Yes or no.	GASI_Farmer, GASI_Field
Farm size	C	Total farm size [ha]	GASI_Farmer
Field size	C	Field size [ha]	GASI_Farmer
Liming	F(2)	Regular liming? Yes or no	GASI_Farmer
Maize	C	Share of maize in crop rotation [-]	GASI_Farmer
Canola, beet and legumes	C	Share of canola, sugar beet and legumes in crop rotation [-]	GASI_Farmer
Livestock	C	Livestock units. One livestock unit represents 500 kilogrammes of farm animals. Calculated in accordance with the Kuratorium für Technik und Bauwesen in der Landwirtschaft e. V. (KTBL), Darmstadt	GASI_Farmer
Livestock per ha	C	Livestock units divided by total farm size	GASI_Farmer
Land-use	F(3)	Land use: annual crops, perennial crops or grassland	GASI_Farmer, GASI_Field
Soil transport	F(3)	No soil transportation, soil accumulation (deposition) or abrasion (erosion)	GASI_Field
Deep chiselling	F(2)	Deep chiselling? Yes or no.	GASI_Farmer
Deep ploughed	F(2)	Deep ploughed? Yes or no.	GASI_Farmer, GASI_Field
Soil			
C/N ratio	C	Ratio of soil organic carbon to total nitrogen [-]. Statistic for predicting physicochemical melioration: mean (0-100 cm)	GASI_Lab
EC	C	Electric conductivity (1:5) [µS cm^{-1}] . Statistic for predicting physicochemical melioration: mean (0-100 cm)	GASI_Lab
PD	C	Packing density [g cm^{-3}] . Statistic for predicting physicochemical melioration: max (0-100 cm)	Schneider, F. & Don, A. (submitted)
Biopores	C	Biopore abundance [vol-%]. Statistic for predicting physicochemical melioration: mean (0-100 cm)	GASI_Field
Munsell chroma	C	Soil colour - purity (chroma) according to Munsell colour system [-]. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Field
Munsell value	C	Soil colour - lightness (value) according to Munsell colour system [-]. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Field
Oximorphic features	C	Area percentage of oximorphic features at profile wall. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Field
Reductomorphic features	C	Area percentage of redoximorphic features at profile wall. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Field
Stagnogleyic horizon	C	Area percentage with stagnogleyic soil horizon. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Field
Boulders	C	Boulder sized rock fragments [vol-%]. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Field
Soil order	F(3)	Bodenabteilung (Engl. great soil group) classified according to AD-HOC-AG Boden (2005).	GASI_Field
Groundwater	F(8)	Depth to groundwater table. Levels according to AD-HOC-AG Boden (2005).	GASI_Field
pH	C	pH measured in deionized water (1:5). Statistic for predicting physicochemical melioration: min (0-100 cm).	GASI_Lab
RRL: acidity	F(6)	Root restriction due to acidity. Statistic for predicting physicochemical melioration: max (0-100 cm).	Schneider, F. & Don, A. (submitted)
RRL: anoxia	F(5)	Root restriction due to anoxia. Statistic for predicting physicochemical melioration: max (0-100 cm).	Schneider, F. & Don, A. (submitted)
RRL: cement	F(5)	Root restriction due to cementation. Statistic for predicting physicochemical melioration: max (0-100 cm).	Schneider, F. & Don, A. (submitted)
RRL: compacted	F(6)	Root restriction due to compactness. Statistic for predicting physicochemical melioration: max (0-100 cm).	Schneider, F. & Don, A. (submitted)
RRL: depth	F(5)	Root restriction due to consolidated bedrock. Statistic for predicting physicochemical melioration: max (0-100 cm).	Schneider, F. & Don, A. (submitted)
RRL: gravel	F(5)	Root restriction due to rock fragments. Statistic for predicting physicochemical melioration: max (0-100 cm).	Schneider, F. & Don, A. (submitted)
RRL: sandy subsoil	F(4)	Root restriction due to sandy subsoil. Statistic for predicting physicochemical melioration: max (0-100 cm).	Schneider, F. & Don, A. (submitted)
RRL: total	F(6)	Root restriction due to acidity, anoxia, cementation, compactness, bedrock, rocks and/or sandy subsoil	Schneider, F. & Don, A. (submitted)
Silt	C	Silt [mass-% of fine soil < 2mm]. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Lab
Rock fragments	C	Rock fragments [vol-%]. Statistic for predicting physicochemical melioration: max (0-100 cm).	GASI_Lab
TIC	C	Total inorganic carbon [mass-% of fine soil < 2mm]. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Lab
SOC	C	Total organic carbon [mass-% of fine soil < 2mm]. Statistic for predicting physicochemical melioration: mean (0-100 cm).	GASI_Lab

* C = continuous variable; F(L) = categorical variable with L levels

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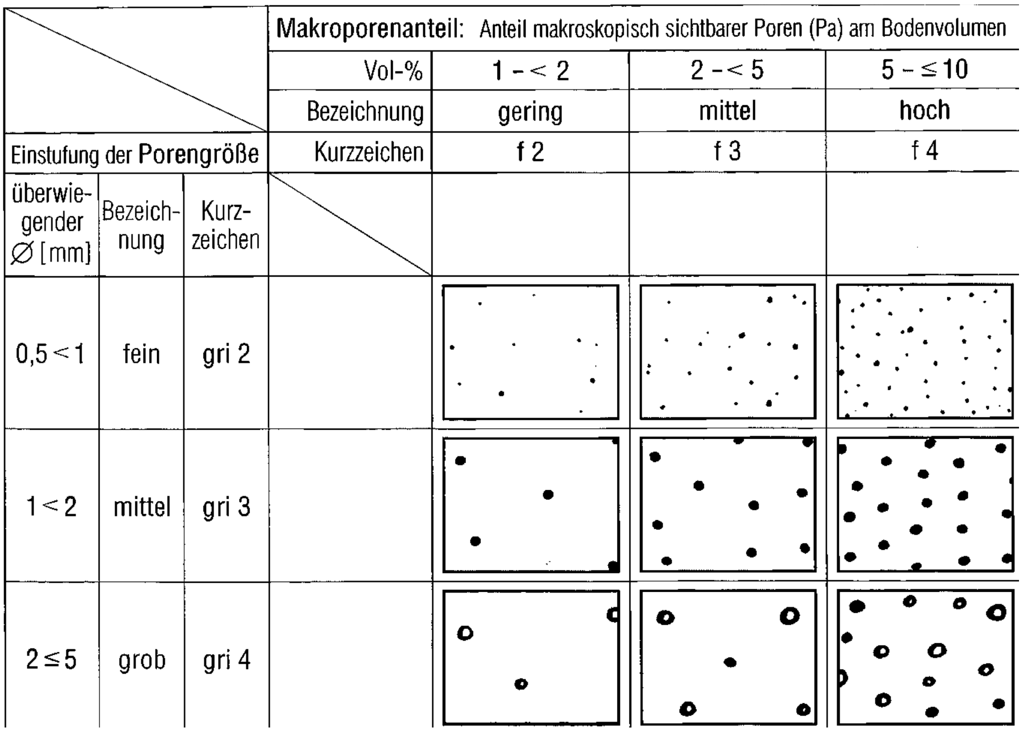
BGR_BAG5000	Bundesanstalt für Geowissenschaften und Rohstoffe: BAG5000 V3.0, Hannover, 2007
BGR_BÜK200	Bundesanstalt für Geowissenschaften und Rohstoffe: BÜK200, Hannover, 2018
BGR_GMK1000	Bundesanstalt für Geowissenschaften und Rohstoffe: GMK1000R V2.0, Hannover, 2006
BKG_NUTS	Bundesamt für Kartographie und Geodäsie: Verwaltungsgebiete 1 : 25 0000 (http://www.bkg.bund.de), 2017
BKG_DGM25	Bundesamt für Kartographie und Geodäsie: Digitales Geländemodel Gitterweite 25 m (http://www.bkg.bund.de), 2018
DWD_Precip.mean	DWD Climate Data Centre (CDC): Multi-annual grids of precipitation height over Germany 1981-2010, v1.0, 2017
DWD_Sun	DWD Climate Data Center (CDC): Multi-annual grids of annual sunshine duration over Germany 1981-2010, v1.0, 2017
DWD_Temp.min	DWD Climate Data Center (CDC): Multi-annual grids of monthly averaged daily minimum air temperature
GASI_Farmer	German Agricultural Soil Inventory: Farmer questionnaire.
GASI_Field	German Agricultural Soil Inventory: Soil profile descriptions by field workers.
GASI_Lab	German Agricultural Soil Inventory: Laboratory
Jacobs, A. et al. (2018)	Jacobs, A., Flessa, H., Don, A., Heidkamp, A., Prietz, R., Dechow, R., Gensior, A., Poeplau, C., Riggers, C., Schneider, F., Tiemeyer, B., Vos, C., Wittnebel, M., Müller, T., Säurich, A., Fahrion-Nitschke, A., Gebbert, S., Hopstock, R., Jaconi, A., Kolata, H., Lorbeer, M., Schröder, J., Laggner, A., Weiser, C., Freibauer, A., 2018. Landwirtschaftlich genutzte Böden in Deutschland – Ergebnisse der Bodenzustandserhebung. Thünen Institut, Braunschweig.
Gebbert, S. (unpublished)	Derived from Landsat (NASA, USGS) images
Roßberg, D. et al. (2007)	Roßberg, D., Michel, V., Graf, R., Neukampf, R., 2007. Definition von Boden-Klima-Räumen für die Bundesrepublik Deutschland. Nachrichtenblatt des deutschen Pflanzenschutzdienstes 59, 155-161.
(Schneider and Don submitted)	Schneider, F. & Don, A. (submitted). Root restricting layers in German agricultural soils. Part I: Extent and cause.

Table C.2: Conversion of biopore classes to continuous scale.

Classes based on AD-HOC-AG Boden (2005)		Present study
Category	Range	Value
[-]	Vol-%	
-	-	0
f1	< 1	0.5
f2	1 to < 2	1.5
f3	2 to < 5	3.5
f4	5 to < 10	7.5
f5	10 to < 30	20
f6	30 to < 50	40



Einstufung der Porengröße			Makroporenanteil: Anteil makroskopisch sichtbarer Poren (Pa) am Bodenvolumen			
			Vol-%	1 - < 2	2 - < 5	5 - ≤ 10
			Bezeichnung	gering	mittel	hoch
			Kurzzeichen	f 2	f 3	f 4
überwiegender ∅ [mm]	Bezeichnung	Kurzzeichen				
0,5 < 1	fein	gri 2				
1 < 2	mittel	gri 3				
2 ≤ 5	grob	gri 4				

Figure C.1: Field chart for estimating ordinal abundance classes of biopores after AD-HOC-AG Boden (2005).

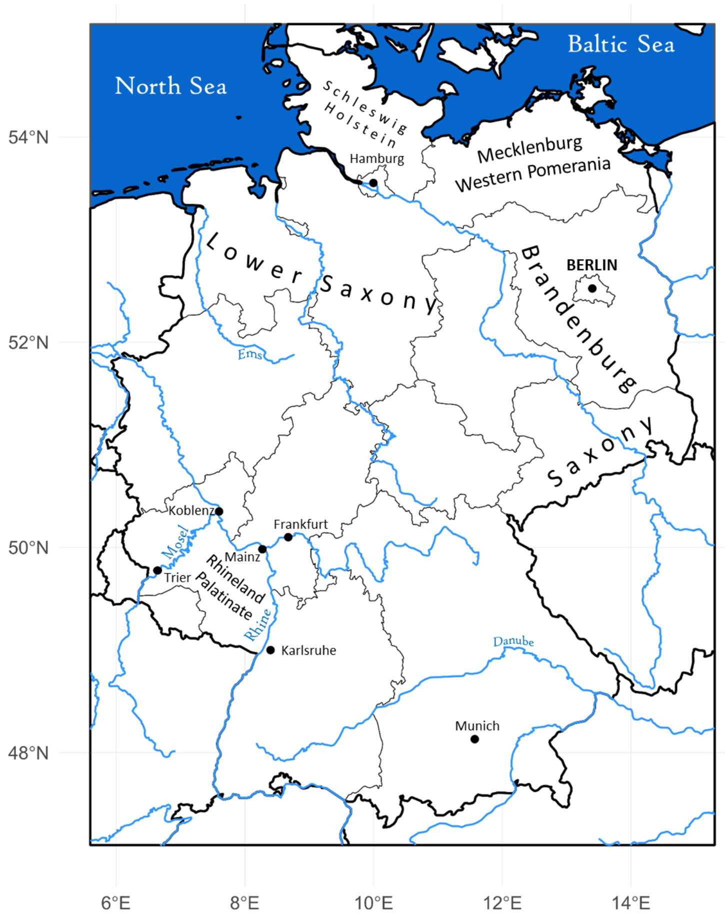


Figure C.2: Map of Germany. Made with Natural Earth (`www.naturalearthdata.com`).

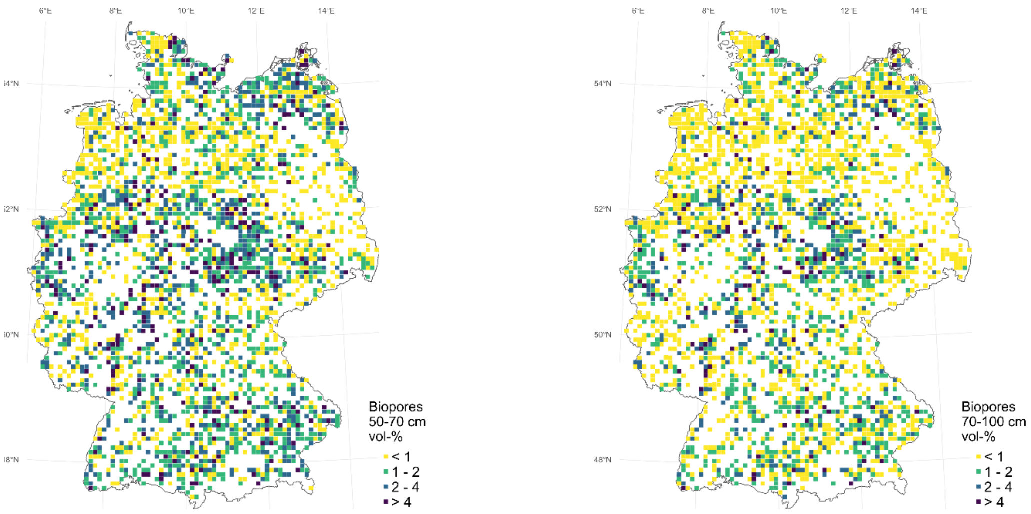


Figure C.3: Biopore abundance in German agricultural soils at 50–70 cm (left) and 70–100 cm depth (right).

Appendix D

▷ Chapter 5

Table D.1: Area estimates for meliorative deep tillage in Germany.

Study*	Soil	Method of deep tillage	Area extent [ha]	Explanation
Eggelsmann (1979)	Podzols and raised bogs	Deep ploughing	245,000	
	Luvisols	Deep ploughing	110,000	
Foerster (1974)	Podzols	Deep ploughing	30,000	Estimate only refers to Weser-Ems area in north-west Germany from 1950 to 1975
Gehrt (2012)	Sandy soils – asparagus cultivation	Mixing	15,000	Estimate only refers to Niedersachsen, north-west Germany
	Sandy soil	Deep ploughing	64,000	
	Loamy soil	Deep ploughing	86,000	
	Peatland	Deep ploughing	89,000	
Kuntze (1974)	Raised bogs	Deep ploughing	120,000	
Kuntze (1986)	Podzols	Deep ploughing	400,000	
	Stagnosols	Subsoiling	100,000	
Renger (1974)	Sandy soils	Deep ploughing + deep placement of manure	50,000	Estimate only refers to eastern Germany

* Citations:
Eggelsmann, R., 1979. Vom Dampfpflug zum Tiefkulturpflug —Entwicklung und Einsatz. Z. f. Kulturtechnik und Flurbereinigung 20, 99—112.
Foerster, P., 1974. Ergebnisse des Tiefpflügens in Sandböden Norddeutschlands. Landbauforschung Völkenrode, Sonderheft 24, 47-68.
Gehrt, E., 2012. Kultosole in Niedersachsen - Merkmale und Verbreitung. Presentation on DBG Tagung, Kommission V, Berlin.
Kuntze, H., 1974. Meliorationsbeispiel Sandmischkultur. Landbauforschung Völkenrode, Sonderheft 24, 31-45.
Kuntze, H., 1986. Soil reclamation, improvement, recultivation and conservation in Germany. Zeitschrift für Pflanzenernährung und Bodenkunde 149, 500-512.
Renger, M., 1974. Bodenkundliche Kriterien für die Auswahl von Verfahren der Tiefenbearbeitung auf meliorationsbedürftigen Standorten. Landbauforschung Völkenrode, Sonderheft 24, 1-14.

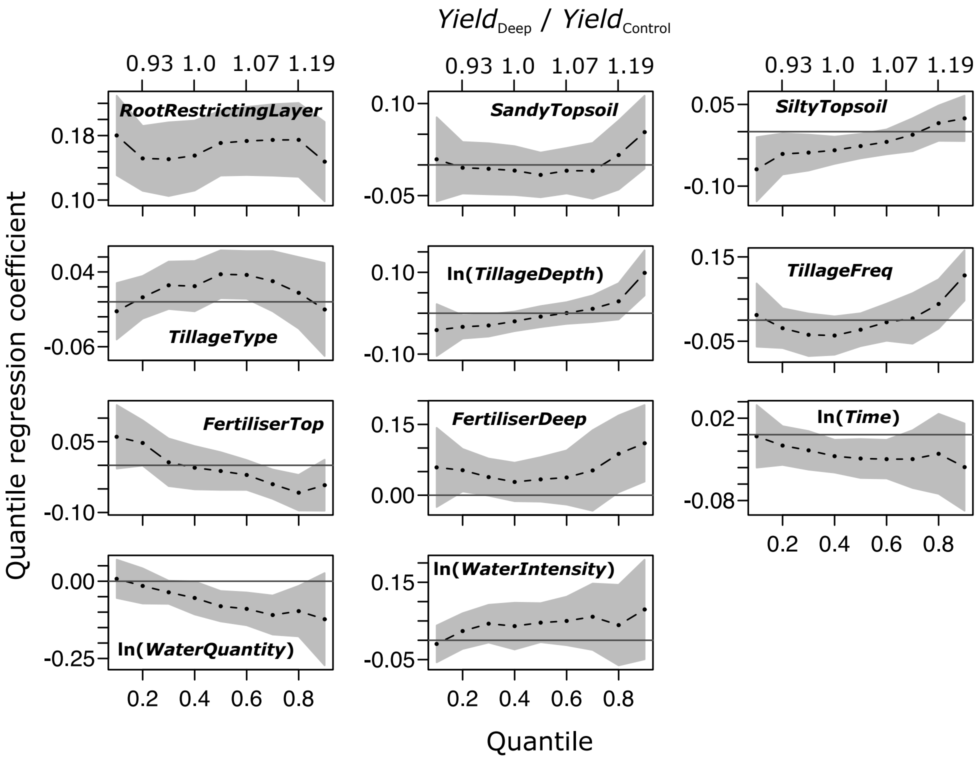


Figure D.1: Effect of site properties (*RootRestrictingLayer*, *SandyTopsoil*, *SiltyTopsoil*), management regime (*TillageType*, ln(*TillageDepth*), *TillageFreq*, *FertiliserTop*, *FertiliserDeep*, ln(*Time*)) and water availability (ln(*WaterQuantity*), ln(*WaterIntensity*)) on the conditional distribution of deep tillage effects expressed as quantile regression coefficients. Grey bands depict point-wise 90% confidence intervals based on bootstrap quantiles clustered by studies.

Danksagungen

An dieser Stelle möchte ich vor allem den Folgenden danken, ohne die die vorliegende Arbeit weder möglich gewesen wäre noch Spaß bereitet hätte:

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Thank you :)