Digital soil mapping for modelling of transport pathways for pesticides to surface water

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Förord
Denna rapport bygger på resultat från projektet *Transport pathways for pesticides to surface water* (SLFH1133108) vilket finansierades av Stiftelsen Lantbruksforskning. Målet med denna del av projektet var att ta fram detaljerade, digitala markkartor på textur (sand- och lerhalt) och mullhalt som skulle kunna användas för spatial modellering av läckage av olika typer av pesticider.

Rapporten är på engelska med en svensk sammanfattning.

Trevlig läsning
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Sammanfattning

Det som redovisas i den här rapporten utgör den första delen av projektet Spridningsvägar för kemiska bekämpningsmedel till ytvatten (SLFH1133108), som finansieras Stiftelsen Lantbruksforskning. Syftet är att ta fram detaljerade digitala kartor över textur (ler- och sandhalt) och mullhalt i matjord och alv. De framtagna kartorna skall sedan användas för rumslig modellering av trasportvägar för olika typer av bekämpningsmedel från åkermark till ytvatten.

Digital markkartering


Högupplösta bakgrundsdata

Högupplösta textur- och mullhaltskartor togs fram för för tre djup i markprofilen. Vi använde tre olika typer av proximala marksensorer (Figur 3) i kombination med en kvartärgeologisk karta (Sveriges geologiska undersökning) och och en laserskannad höjdmodell (Lantmäteriet).

Jordprover

I matjorden togs 84 jordprover och i alven togs 18 prover. Dessa analyserades för textur (sedimentationsmetoden) och mullhalt (glödförlustmetoden) på Institutionen för mark- och miljö vid Sveriges lantbruksuniversitet.

Karterade markegenskaper

Vi tog fram kartor för tre olika djup: matjorden (0-0.2 m djup), övre delen av alven (0.2-0.45 m djup) och den djupa alven (0.45-0.7 m djup). De markegenskaper som karterades var lerhalt (partikelstorlek < 2 µm, Figur 2), sandhalt (partikelstorlek 0.2 - 2 mm) och mullhalt. Mullhalten delades in i fyra klasser: låg (u: < 3 % mull), mellan (n: 3 - 5 % mull), hög (h: ≤5 % mull) samt torvjordar (t).

Modellering

Olika modelleringstrategier testades och den strategi som fungerade bäst för varje markegenskap och djupintervall användes för att ta fram de slutliga kartorna. Den bästa metoden var i samtliga fall att ta fram kartornagenom Marsplines-modellering (Hastie et al., 2009).

Validering

Genom att undanhålla ett jordprov i taget och ta fram nya kartor (s.k. korsvalidering) kunde vi få ett mått på hur bra karteringsmetoden fungerar. Absolut medelfel och andel korrekt klassificerade mullhalter redovisas i Figur 5 och Figur 7.

Beskrivning av området

Karteringen visar att det är stor variation i både textur och mullhalt i de karterade delavrinningsområdena. I jordproven varierade lerhalten mellan 5 % och 52 % i matjorden. I vissa områden, men inte överallt, ökade lerhalten något neråt i markprofilen. Mullhalten
Summary

Detailed spatial information of soil texture and SOM content are needed for the modelling of pesticide fate. As part of the SLF project *Transport pathways for pesticides to surface water* (SLFH1133108) such maps were derived for three depth layers of the soil profile in two sub-catchments with a total area of 450 ha. Data from proximal sensor measurements were combined with national datasets (a digital elevation model and a Quaternary deposit map) and calibrated against soil sample data. Different modelling strategies were tested and the best strategy for each layer was selected for production of the final maps. For topsoil texture, Marsplines modelling with a reduced number of covariables gave the best results (the final models included topographic variables and gamma radiation). In the upper subsoil, the texture was best predicted by an empirical relationship to the topsoil predictions. This is not surprising since the number of calibration samples in the subsoil was very small (n = 18) compared to the number of calibration samples (n = 85). In the deep subsoil, the best strategy was again to use Marsplines modelling with a reduced number of covariables. The SOM content in the topsoil and was mapped by Marsplines modelling using a limited number of predictors and allowing interactions. In the subsoil, however, all soil samples but one had SOM < 3 % and the entire area was classified as as SOM class u. Organic soils according to the SGU QD map (peat areas) were not included in the mapping. Instead they were directly assigned as SOM class t and the texture was not determined.
Introduction

What is presently reported, forms part of the project *Transport pathways for pesticides to surface water* (SLFH1133108) funded by The Swedish Farmers’ Foundation for Agricultural Research. The aim of this part was to derive detailed digital soil maps of texture (fractions of clay and sand) and soil organic matter content (SOM) to be used in spatial modelling of leaching pathways of different types of pesticides.

To derive high resolution maps solely based on laboratory analyses of soil samples would be an expensive and time-consuming task. Therefore, more efficient strategies have been developed. Digital soil mapping (DSM) refers to methods to derive high resolution digital soil maps from a combination of exhaustive ancillary variables and calibration data from laboratory analyses of soil samples (Figure 1). The ancillary variables are also known as predictor variables, predictors, covariables or X variables and the response variable, i.e. the variable to be mapped, is also known as the target variable or the Y variable. The soil samples are used to calibrate a prediction model that is subsequently deployed on the exhaustive covariable dataset to derive a map of the target variable.

An important part of the work is to validate the method and it is essential to do so at a relevant scale. A model that performs poorly within a field might still capture the variation at the regional scale well; regional validation says little about the model performance within a watershed or a single field. The risk of making nice-looking but non-realistic maps is also lessened if the predictor data used are actually related to the target variable, and have an accuracy that allows for mapping at the intended spatial resolution. McBratney et al. (2003) was early to outline the principles for good DSM practices.

In this study, we used a combination of proximally and remotely sensed covariables. Proximal sensors are efficient tools to rapidly collect high resolution spatial data within agricultural fields and there is a multitude of measurement techniques, traditionally used in laboratories, that has been modified for use *in situ* (Viscarra Rossel et al., 2011). For the present project we used proximal *in situ* measurements of apparent electrical conductivity (ECa) and natural gamma radiation (isotopes: $^{40}$K, $^{232}$Th and $^{238}$U). ECa is affected by soil type and moisture conditions and is often correlated to yield (Van Meirvenne et al., 2013). Measurements of the naturally occurring isotope $^{232}$Th have been demonstrated to be a good predictor of clay content (van der Klooster et al., 2011). Elevation and relative topography were used as covariables since some soil forming processes are governed by topography. However, Odeh et al. (1994) found that the use of landform attributes as covariables improved interpolation of subsoil clay content but neither Taylor et al. (2010) nor (Piikki et al., 2013) found elevation data to be useful as covariables for texture predictions. In addition to measured data, we also included legacy map data in the covariable set from a national Quaternary deposit map. The methods for modelling and data analyses followed the procedures described in Söderström et al. (2015).
Materials and methods

Map area

Two sub catchments in the E21 area for environmental monitoring, together covering 450 ha, were mapped. Raster maps of 10 m × 10 m were prepared for each of three depth layers, 0-20 cm, 20-45 cm and 45 -70 cm.

Soil samples

Point locations were selected by random stratification, n = 85 in the topsoil and n = 18 in each of the two subsoil layers. Four subsamples were taken at each depth interval and pooled to one sample. The subsamples were taken with a 0.5 m radius. The texture was analyzed with the sedimentation method (Method: ISO 11277) and the SOM content was determined by loss on ignition (original method by Ekström, 1927) at the laboratory at the Department of Soil and Environment, SLU, Sweden.

Sensor data

Measurements were made in the field with two different proximal sensors (Figure 2). Natural emissions of gamma radiation from $^{40}$K, $^{232}$Th and $^{238}$U were measured with a vehicle-borne gamma spectrometer (The Mole, The Soil Company, The Netherlands). Also the total count of decays (TC) and the ratios among the isotopes were used as predictors. The measurements were done along tracks 24 m apart.

The ECa was measured over two different depth intervals, using an electromagnetic induction sensor with two reception coils (EM38 mk2, Geonics Ltd, Canada). The instrument was dragged by a four wheel motorbike across the fields. Like the radiometric measurements, readings were taken along tracks 24 m apart. In 76 ha of the area, a web of cupper (Cu) cables was buried in the soil, a remnant earth connection of a former radio station. The highly conductive cupper caused the electromagnetic induction measurements to fail. Instead, the soil electrical conductivity was measured with a dipole probe (Veris P4000, Veris Technologies, USA) at 21 point locations in this area (Figure 2 c).
**Elevation data**

Elevation data were extracted from the Grid 2+ database (Swedish Land Survey) and aggregated to 10 m × 10 m resolution, which was considered more appropriate for this work and also easier to handle than the original 2 m × 2 m resolution. The relative topography (RT; Equation 1) was calculated in three different neighborhoods of sizes 5 ha, 50 ha and 500 ha.

\[
RT = \text{raster cell elevation} - \text{average neighborhood elevation}
\]  

**(Equation 1)**

**Quaternary deposit map**

Data from the 1:50 K Quaternary deposit (QD) map (The geological survey of Sweden, SGU) were reclassified into 

1. five classes (clay, organic sand, till and till clay) and
2. three classes (clay, organic and other).

This may seem like creating redundant information but since the data mining method used in the present study do not force all variables into the model, but excludes any variables that do not contribute to a better model performance, it was possible to include both classification versions and let the best be selected in the parameterization.

**Target variables**

Texture (fractions of clay and sand) and soil organic matter content (SOM). Clay (particle size < 2 µm) and sand (particle size 0.06 - 2 mm) are expressed as fractions of the fine soil (particle size < 2 mm). To match the pesticide model requirements, the SOM content was classified as follows:

- u: Low organic carbon content (SOM < 3 %);
- n: Medium organic carbon content (3 % ≤ SOM < 5 %);
- h: High organic carbon content (5 % ≤ SOM);
- t: Peat or organic parent-materials.

**Data management**

All predictor data was prepared as 10 m × 10 m rasters using ArcMap 10.1 (Esri Inc., USA) and then transferred to a 10 m × 10 m point grid, which was stored as a text file with coordinates and covariable values, and imported to the statistical software R (R Core Team, 2013). A text file with covariable and target variable values was likewise prepared for the soil sample locations and imported to R. The data for the soil sample locations were used for the calibration of Marsplines models that then were deployed on the grid dataset to create maps. The cross-validation results were imported to Microsoft Excel for further processing, and the prediction rasters were imported to ArcMap, for the visualization of results.

Before any predictive modelling was done, areas where the Quaternary soil class was organic soil were removed. These areas were directly classified as SOM class t (see specifications above) and were left to have missing values for the fractions of clay and sand. This way of handling soils with a high SOM was chosen because, in the laboratory, texture is not determined for samples with a SOM content > 40 %.
Figure 2. The proximal sensors a) EM38 MK2 (Geonics Ltd, Canada) registers the apparent electrical conductivity (ECa) of the soil. Two differently depth-weighted average values of ECa are obtained at each measurement location. b) The Mole (The Soil Company, The Netherlands) registers gamma radiation from the soil. The radiation from three naturally occurring isotopes, $^{40}\text{K}$, $^{232}\text{Th}$ and $^{238}\text{U}$, can be quantified. c) tractor-mounted P 4000 VIS-NIR-EC-Force sensor system (Veris Technologies Inc. USA). ECa profiles measured with the dipole probe was recalculated to depth weighted ECa values and combined with the EM38 data. De proximala sensorerna a) EM38 MK2 (Geonics Ltd, Canada) som registrerar markens elektriska konduktivitet (ECa). Två värden med olika djuprespons erhålls vid varje mätning. b) Mullvaden (The Mole; The Soil Company, The Netherlands) registrerar gammastrålning från marken. Strålningen från tre naturligt förekommande isotoper kan mätas, $^{40}\text{K}$, $^{232}\text{Th}$ och $^{238}\text{U}$. c) det traktorburna sensorsystemet P 4000 VIS-NIR-EC-Force (Veris Technologies Inc. USA). ECa-profiler mätta med systemets prob räknades om till ECa-värden med samma djuprespons som EM38-värdena och användes för att komplettera dessa.

The modelling method

The covariables were calibrated against the soil sample reference data, using multivariate adaptive regression splines (Marsplines; Hastie et al., 2009). A Marsplines model consists of piecewise linear regression models (basis functions), which are valid within defined intervals of the X variables, delimited by break points. One can parameterize simple additive models but pairwise or higher-order interactions among the basis functions are also possible to include. A benefit of the parameterization procedure is that it includes a pruning pass that removes unnecessary basis functions and improves the robustness of the model. Another advantage of Marsplines, compared to some other data mining methods, is the possibility to combine quantitative and qualitative covariables, like elevation (continuous) and soil class (categorical). We used the Earth package in R (Milborrow, 2015) for the parameterization and deployment of Marsplines models. Continuous Marsplines predictions were made also for the categorical target variable (SOM) and the values were afterwards categorized into the u, n and h classes.
**Model parameterizations**

Even with the pruning procedure, there is still a risk of parameterizing overfitted non-robust models. This risk is larger when a larger number of covariables are provided. Therefore, we tested two different sets of covariables, one set with all available covariables and one reduced set. The smaller set consisted of the same covariables as was used for regional mapping in another ongoing DSM project (Söderström et al., 2015).

**Small covariable set:** Soil class (two variables), elevation (one variable), relative topography (three variables) and radioactive isotopes (two variables, $^{232}$Th and $^{40}$K).

**Full covariable set:** Soil class (two variables), elevation (one variable), relative topography (three variables), radioactive isotopes and isotope ratios (seven variables) and ECa (two variables).

Models based on the small predictor set were parameterized with and without interactions and models using the full predictor set were only parameterized without interactions.

In the topsoil, where there were many calibration points (Table 1), it was also tested how well the area could be mapped without any covariables at all, by merely interpolating the calibration data. This was done by ordinary kriging (Isaaks and Srivastava, 1989) for clay and sand. Since there were so many calibration samples in the topsoil and so few in the subsoil, it was tested whether adding the predicted values of topsoil clay and topsoil sand content to predictor set 1 when modelling of the subsoil could improve the predictions.

To sum up, four different strategies (Figure 3) were tested and compared for each depth layer and only the best one for each target variable was used to produce the maps for the pesticide leaching models. After selecting the best mapping strategy for each target variable and depth layer, a final model was calibrated using all calibration points and that model was deployed on the grid data to create the final maps.

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1 An overfitted model is a model that has parameterized not only the functional relationships between the predictors and the target variables, but also the random variation (the noise) in the calibration dataset. Such models describe the variation in the calibration well but do not work well in other areas. A model that captures only general relationships and works well on new data is said to be robust.
The validation procedure

The predicted maps were validated by leave-one-out cross validation. That means that the target variable is predicted at each soil sample location by calibrating a new model with that sample left out. To enable comparison of the four mapping strategies and choose the best models to use for map production, three simple validation measures were calculated. For the texture variables, the coefficient of determination ($r^2$) and the mean absolute error (MAE) were calculated. The $r^2$ value is a measure of how strong a linear relationship between the predicted and the measured values is, while the MAE is the average magnitude of the error, irrespective of whether there is an over-prediction or an under-prediction. For the categorical SOM predictions, the true positive rate (TPR) was calculated instead. TPR is the proportion of the validation points that are classified correctly as SOM class u, n or h (see classification på sidan 9).

Results and discussion

Descriptive statistics

In the topsoil, 85 soil samples were analyzed and they showed a large variation range in all three target soil properties. In the subsoil, fewer samples were taken ($n = 18$). There is a general tendency towards finer particle sizes (higher clay content/lower sand content) in the deeper subsoil compared to the upper part of the soil profile, but there was no consistent pattern among the individual profiles (Figure 4). There is very little SOM in the subsoil; only seven of the 18 samples in the deep subsoil had a detectable SOM content and all of them were of SOM class u ($< 3\%$ SOM; Figure 4 c).
Table 1. Descriptive statistics of the calibration data. n = number of samples in the non-organic part of the watersheds. stdev = standard deviation and SOM = soil organic matter. Statistik för kalibreringsdata. n= antal prov; stdev= standardavvikelse; SOM = mullhalt

<table>
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<th>Variable</th>
<th>n</th>
<th>min</th>
<th>median</th>
<th>mean</th>
<th>max</th>
<th>stdev</th>
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<tr>
<td>(0-20 cm depth)</td>
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<td>58.3</td>
<td>86</td>
<td>15.2</td>
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<tr>
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<td>2.8</td>
<td>3.6</td>
<td>19.6</td>
<td>2.9</td>
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<tr>
<td>(20-45 cm depth)</td>
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<tr>
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<td><strong>Deeper subsoil</strong></td>
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<td>(45-70 cm depth)</td>
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<tr>
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<td>42.7</td>
<td>93</td>
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</tr>
<tr>
<td>SOM</td>
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<td>0.4</td>
<td>0.5</td>
<td>0.8</td>
<td>0.2</td>
</tr>
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</table>

1) The value within parenthesis indicates the number of non-zero values. The zero values were excluded from the statistics.

**Comparison of the mapping strategies**

The validation measures for texture are presented in Figure 5 and topsoil maps of clay content produced with the different mapping strategies are presented in Figure 6. The validation measures for SOM are presented in Figure 7. Concerning topsoil texture, there was not a large difference in the performance between the four tested methods. That may be due to the fact that the datasets available for prediction (lab analyses for and covariable maps for deployment) were good enough for any of the methods to translate it to the target variables. A general trend is that the prediction accuracy decreases for each depth layer downwards in the profile and is least good in the deep subsoil. This is expected since the number of calibration samples is much lower in the subsoil (n = 18) than in the topsoil (n = 84). In addition, the measurements of the most important covariables (the radioactivities of naturally occurring isotopes) are not sensitive to subsoil conditions (Taylor et al., 2002). In the upper subsoil layer, the best mapping strategy was to use the covariable set with few variables and include topsoil predictions. In fact, the parameterized models included only the predicted topsoil texture variables. This is not surprising since, as seen in Figure 4 and Table 1, there is not a considerable difference in texture between the topsoil and the upper subsoil. In the deeper subsoil layer, using Marsplines models with the small set of covariables was judged to be the best strategy.
One outlying point was removed from the clay content cross validations in the deepest soil layer. In this point, the measured clay content was 61% but the predicted value was only about 4% clay in two of the mapping strategies. This may suggest that the measured clay content value for this sample was erroneous, but this can also happen in cross-validation of calibrations with few samples; when a sample that is taken at a location with deviating conditions is removed, the model will not be parameterized to make predictions under such conditions and the prediction for that sample may have a large error. However, in the final map the prediction at the location for the removed outlier was not that erroneous; the predicted clay content by the Marsplines model with few variables was 39%.

For SOM content in the topsoil, the best method was Marsplines predictions using the small covariable set and allowing interactions followed by classification of the continuous predictions. Potassium-40 was an important predictor in the model and there were interactions between $^{40}$K and soil class sand (reclassification of the QD map) and between $^{40}$K and relative topography at the intermediate scale (Figure 8b).

It shall be noted that the strategy to include all predictors and let the model parameterization choose which covariables to include in the model was never the best performing strategy (Figure 5). This highlights the importance of thoroughly considering the addition of each covariable. Adding non-functional predictors just adds noise and increase the risk of
overfitting. It is neither useful to add several functional but highly correlated predictor variables. The parameterization procedure starts with successive addition of new basis functions, based on best improvement of the model, until a predefined number of basis functions are included. If two correlated variables are provided and one is added to the model, it is likely that the second (possibly more relevant) predictor variable never will enter the model (Milborrow, 2015).

In the subsoil, all samples with a detectable SOM content were of SOM class u. It was not possible to create any reliable maps based on this dataset and both subsoil layers were classified as SOM class u over the entire area, except for the areas of SOM class t delineated based on the organic soils in the QD map (see class limits på sidan 9).

The final maps
In the topsoil, Marsplines models with the small set of provided covariables were chosen because of best performance for the clay content predictions (higher $r^2$; Figure 5a). For sand, kriging performed somewhat better but since the difference in performance was not very large, Marsplines with the few covariables was chosen also for this texture parameter in order to get the same spatial variation structure in the final maps of the two texture variables. In the upper subsoil Marsplines models with the topsoil predictions as the only covariable were chosen and in the deep subsoil, Marsplines models parameterized with the few covariables was again chosen for both sand and clay, based on best performance. The final texture subsoil maps passed on to the pesticide fate modelling are presented in Figure 9. As mentioned above the topsoil SOM content was predicted by classification of Marsplines predictions allowing interactions among the covariables and the subsoil SOM was classified as class u over the entire area.
Figure 5. Cross-validation results for the four prediction strategies for texture in a-b) the topsoil, c-d) the upper subsoil and e-f) the deeper subsoil. $r^2 =$ coefficient of determination. MAE = mean absolute error. The modelling strategies used for the final maps are marked with stars. One outlying point was removed from the clay content cross validations in the deepest soil layer.

It is obvious from the topsoil maps that although the variation is about equally well captured at the catchment scale, the maps look rather different within individual farms. The spatial
variation structure of the kriged maps (Figure 6 a) differ from that of the maps produced with covariables (Figure 6 b-d); kriging yields maps with a smoother spatial pattern. The more cluttered patterns of the covariable-derived maps give the impression that these are more accurate at the within-field scale but it is not possible to know whether that is true without a validation sample set collected at this scale (within a field).

Figure 6. Maps of topsoil clay content produced by the four mapping strategies. a) ordinary kriging, b) Marsplines with few covariables, c) Marsplines with many covariables and d) Marsplines with few covariables and interactions. The covariables included in the parameterized Marsplines models are listed. RT = relative topography, ECa= apparent electrical conductivity. The star marks the final map passed on to the pesticide fate modelling.
Figure 7. Cross-validation results for the four prediction strategies for soil organic matter content (SOM) in the topsoil. The modelling strategy used for the final maps is marked with a star. The true positive rate is the proportion of the validation points that are classified correctly as SOM class u, n or h (see classification on page 4).

Figure 8. Final maps passed on to the pesticide fate modelling of a) topsoil sand content and b) soil organic matter (SOM) content. The covariables included in the parameterized models are listed. RT = relative topography, ECa = apparent electrical conductivity. u = low organic carbon content (SOM < 3 %); n = medium organic carbon content (3 % ≤ SOM < 5 %); h: High organic carbon content (SOM ≥ 5 %).
Figure 9. The final maps of texture in the two subsoil layers a-b) 20-45 cm depth and c-d) 45-70 cm depth. The maps were produced by the methods indicated by stars in Figure 5. The covariables included in the parameterized Marsplines models are listed. RT = relative topography, ECa = apparent electrical conductivity. De slutliga kartorna över ler- och sandhalt i alven a-b) 20-45 cm djup och c-d) 45-70 cm djup. Kartorna har tagits fram med de metoder som markeras med en stjärna i figur 5. De kovaribler som kom med i den kalibrerade modellen listas. RT = relative topografi, ECa= markens elektriska ledningsförmåga.
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1. Rapport från en studieresä till norra Tyskland.
AGROVÄST-projektet Precisionsodling Sverige syftar till att utveckla och tillämpa användbara metoder inom precisionsodlingen till nytta för det praktiska jordbruket.

I projektet arbetas med precisionsodling i form av utvärdering och tolkning av samt teknik för markkartering, kalkning, gödsling, bestämning av mark- och grödegenskaper, växtskydd samt miljöeffekter av precisionsodling.

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