Using Advanced Regression Models for Determining Optimal Soil Heterogeneity Indicators

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Abstract Nowadays in agriculture, with the advent of GPS-based vehicles and 5 sensor-aided fertilization, large amounts of data are collected. With the importance 6 of carrying out effective and sustainable agriculture getting more and more obvious, 7 those data have to be turned into information - clearly a data analysis task.

Furthermore, there are novel soil sensors which might indicate a field's hetero-9 geneity. Those sensors have to be evaluated and their potential usefulness should be 10 assessed. Our approach consists of two stages, of which the first stage is presented 11 in this article. 12

The data attributes will be comparable to the ones described in Ruß (2008). In 13 the first stage, we will build and evaluate models for the given data sets. We will 14 present a comparison between results using neural networks, regression trees and 15 SVM regression. Results for an MLP neural network have been published in Ruß 16 et al. (2008). In a future second stage, we will use the model information to evaluate 17 and classify new sensor data. We will then assess their usefulness for the purpose of 18 (yield) optimization. 19 100

Introduction 1

Due to the modernization and better affordability of state-of-the-art GPS technology 21 and a multitude of available sensors, a farmer nowadays harvests not only crops 22 but also growing amounts of data. These data are small-scale and precise – which 23 is essentially why the combination of GPS, agriculture and data has been termed 24 precision agriculture. 25

However, collecting large amounts of data often is both a blessing and a curse. 26 There is a lot of data available containing information about a certain asset – here: 27 soil and yield properties – which should be used to the farmer's advantage. This is a 28

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common problem for which the term *data mining* or *data analysis* has been coined. 29 Data analysis techniques aim at finding those patterns or information in the data that 30 are both valuable and interesting to the farmer. 31

A common specific problem that occurs is yield prediction. As early into the 32 growing season as possible, a farmer is interested in knowing how much yield he is 33 about to expect. In the past, this yield prediction has usually relied on farmers' 34 long-term experience for specific fields, crops and climate conditions. What if 35 a computational model could be generated that allows to predict current year's 36 yield based on past data and current year data? This problem of yield predic-37 tion encountered here is one which intelligent data analysis should be applied to. 38 More specifically, multi-dimensional regression techniques could be used for yield 39 prediction. 40

Nowadays, we can collect small-scale, precise data in-season using a multitude 41 of sensors. These sensors essentially aim to measure a field's heterogeneity. In future 42 work, these sensors will be assessed as to how useful they are for the purpose of yield 43 prediction. For this work, this article should serve as an overview on the capabilities 44 of different regression techniques used on agricultural yield data. 45

1.1 Research Target

The overall research target is to find those indicators of a field's heterogeneity which 47 are suited best to be used for a yield prediction task. Since this should be done 48 in-season, the sub-task here is one of multi-dimensional regression – predicting 49 yield from past and in-season attributes. At a later stage, when multi-year data are 50 available, models from past years could be used to predict present year's yield. 51

Therefore, this work aims at finding suitable data models that achieve a high 52 accuracy and a high generality in terms of yield prediction capabilities. Since multi-53 year data are not yet available, the prediction can only be done in space using cross-54 validation, instead of in time. As soon as multi-year data are available, the models 55 can be trained using these data for prediction in time. We will evaluate different 56 types of regression techniques on different data sets. Since these models usually are 57 strongly parameterized, an additional question is whether the model parameters can 58 be carried over from one field to other fields which are comparable in (data set) size. 59 This issue will also be addressed in this work. This is especially useful when new 60 data have to be evaluated using one of the presented models. 61

1.2 Article Structure

Section 2 lays out the data sets that this work builds upon. The attributes and 63 their properties will be presented shortly. Section 3 briefly presents four selected 64 regression techniques from the data mining area which will be used for yield 65 prediction. 66

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Section 4 shows the results of the modeling/regression stage and provides ans- 67 wers to the aforementioned research questions. 68

At the end of this article, future work is pointed out and implementation details 69 are provided. 70

2 Data Description

The data available in this work have been obtained in the years 2003–2006 on 72 three fields near Köthen, north of Halle, Germany (GPS coordinates: Latitude N 73 51 40.430, Longitude E 11 58.110). All information available for these 65-, 72- 74 and 32-hectare fields was interpolated using kriging (Stein 1999) to a grid with 10 75 by 10 meters grid cell sizes. Each grid cell represents a record with all available 76 information. During the growing season of 2006, the latter field was subdivided into 77 different strips, where various fertilization strategies were carried out. For an example of various managing strategies, see e.g. Schneider and Wagner (2006), which 79 also shows the economic potential of PA technologies quite clearly. The fields grew 80 winter wheat, where nitrogen fertilizer was distributed over three application times 81 during the growing season.

Overall, for each field there are seven attributes – accompanied by the respective 83 current year's yield (2004 or 2006) as the target attribute. Those attributes have been 84 described in detail in Ruß et al. (2008), an overview is given below. In total, for the 85 F04 field there are 5241 records, for F131 there are 2278 records, for F330 there are 86 4578 records, thereof none with missing values and none with outliers. In addition, 87 a subset for F131 was available: in this subset, a special fertilization strategy was 88 carried out which used a neural network for prediction and optimization – this data 89 set is called F131net and has 1144 records.

In this work, data sets from three different fields are evaluated. A brief summary 91 of two of the available data sets is given in Tables 1a and 1b. On each field, dif-92 ferent fertilization strategies have been used. One of those strategies is based on a 93 technique that uses a multi-layer perceptron (MLP) for prediction and optimization. 94 This technique has been presented and evaluated in, e.g., Ruß et al. (2008); Ruß 95 (2008) or Weigert (2006). For each field, one data set will contain all records, thus 96 containing all the different fertilization strategies. In addition, a subset of F131 has 97 been chosen to serve as a fourth data set to be evaluated. 98

3 Advanced Regression Techniques

As mentioned in the introduction, the task of yield prediction is essentially a task 100 of multi-dimensional regression. Therefore, this section will serve as an overview 101 about different regression techniques that are applicable to the yield data sets. We 102 aim to evaluate these techniques on the data sets presented in the preceding section. 103

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t1.1 Table 1 Overview of the F04 and F131 data sets. The additional data sets F330 and F131net, which is a subset of F131, are not shown as their statistical properties are very similar to those of F04 and F131

t1.2	(a) Data overview, F04				(b) Data overview, F131					
t1.3	F04	min	max	mean	std	F131	min	max	mean	std
t1.4	YIELD03	1.19	12.38	6.27	1.48	yield05	1.69	10.68	5.69	0.93
t1.5	ЕМ38	17.97	86.45	33.82	5.27	EM38	51.58	84.08	62.21	8.60
t1.6	N1	0	100	57.7	13.5	N1	47.70	70	64.32	6.02
t1.7	N2	0	100	39.9	16.4	N2	14.80	100	51.71	15.67
t1.8	N3	0	100	38.5	15.3	N3	0	70	39.65	13.73
t1.9	reip32	721.1	727.2	725.7	0.64	reip32	719.6	724.4	722.6	0.69
1.10	reip49	722.4	729.6	728.1	0.65	reip49	722.3	727.9	725.8	0.95
1.11	vield04	6.42	11.37	9.14	0.73	yield06	1.54	8.83	5.21	0.88

The regression task can be formalized as follows: the training set

$$T = \{\{x_1, \dots, x_n\}, y_i\}_{i=1}^N$$

is considered for the training process, where $x_i, i = 1, ..., n$ are continuous input 105 values and $y_i, i = 1, ..., N$ are continuous output values. Given this training set, 106 the task of the regression techniques is to approximate the underlying function 107 sufficiently well.

3.1 Introduction to Regression Techniques

Since one particular technique, namely MLPs, has been used successfully in previous work (Ruß et al. 2008; Ruß 2008), it is used as a reference model here. Three 111 additional modeling techniques, namely RBF networks, regression trees, and support vector regression, will be presented, which are suitable for the task of yield 113 prediction. The aforementioned techniques have, to the authors' knowledge, not 114 been compared to each other when used with different data sets in the agriculture 115 context. This section presents some of the background for each of the techniques 116 before they will be evaluated in Sect. 4. 117

3.2 Neural Networks

In previous work multi-layer perceptrons (MLPs), a type of neural networks, have 119 been used for a modeling task (Ruß et al. 2008; Ruß 2008) similar to the one 120 encountered here. Furthermore, neural networks have shown to be quite effective 121 in modeling yield of different crops (Drummond et al. 1998; Serele et al. 2000). 122 The MLP model was established as a reference model against which further regres-

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sion techniques would have to compete. For a more detailed and formal description 124 of MLP neural networks, it is referred to Hagan (1995) or Haykin (1998). The network layout and the parameters will be given in Sect. 4. In this work, the matlab 126 implementation for the MLP network was used: newff. 127

Furthermore, a different type of neural network, a radial basis function (RBF) 128 network, will be evaluated, since it is well-suited to the regression task. For this 129 network, matlab's newrb function has been utilized. 130

3.3 Regression Tree

Regression as well as decision trees are usually constructed in a top-down, greedy 132 search approach through the space of possible trees (Mitchell 1997). The basic algo-133 rithms for constructing such trees are CART (Breiman et al. 1984), ID3 (Quinlan 134 1986) and its successor C4.5 (Quinlan 1993). The idea here is to ask the question 135 "which attribute should be tested at the top of the tree?" To answer this question, 136 each attribute is evaluated to determine how well it is suited to split the data. The 137 best attribute is selected and used as the test node. This procedure is repeated for the 138 subtrees. For further information on the construction details and possible problems 139 (such as overlearning) the reader is referred to Mitchell (1997). For this work the 140 standard matlab implementation of classregtree has been utilized.

3.4 Support Vector Regression

Support Vector Machines (SVMs) are a supervised learning method discovered 143 by Boser et al. (1992). However, the task here is regression, so the focus is on support vector regression (SVR). A more in-depth discussion can be found in Gunn 145 (1998). Given the training set, the goal of SVR is to approximate a linear function 146 $f(x) = \langle w, x \rangle + b$ with $w \in \mathbb{R}^N$ and $b \in \mathbb{R}$. This function minimizes an empirical 147 risk function defined as 148

$$R_{emp} = \frac{1}{N} \sum_{i=1}^{N} L_{\varepsilon}(\hat{\mathbf{y}} - f(\mathbf{x})), \qquad (2)$$

where $L_{\varepsilon}(\hat{y} - f(x)) = \max((|\xi| - \varepsilon), 0)$. $|\xi|$ is the so-called slack variable, which 149 has mainly been introduced to deal with otherwise infeasible constraints of the opti-150 mization problem, as has been mentioned in Smola and Schölkopf (1998). By using 151 this variable, errors are basically ignored as long as they are smaller than a prop-152 erly selected ε . L_{ε} is called ε -insensitive loss function. Other kinds of functions 153 can be used, some of which are presented in Chap. 5 of Gunn (1998). To estimate 154 f(x), a quadratic problem must be solved. See Mejía-Guevara and Kuri-Morales 155

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(2007) for the dual form of this problem. In this work, the SVMtorch implementation from Collobert et al. (2001) has been utilized. Its documentation also points out
further details of the SVR process.

3.5 Linear Regression and Naive Estimator

For comparison reasons, two further prediction methods are employed to compare 160 the advanced regression techniques against. The first of these is a simple multilinear regression estimator. The second is a naive estimator which simply reports 162 the previous year's yield as the output yield of the current year. 163

3.6 Model Parameter Estimation

Each of the aforementioned four different models will be evaluated on the same 165 data sets. One of the research goals here is to establish whether a model which has 166 been used on one data set can be used on a different data set without changing 167 its parameters. This would lead us to believe that comparable fields could use the 168 same prediction model. Hence, the F04 data set is used to determine the model 169 parameters experimentally. Afterwards, the models are re-trained on the remaining 170 data sets using the settings determined for F04. The parameter settings are given in 171 Sect. 4.

For training the models, a cross-validation approach is taken. As mentioned in 173 e.g. Hecht-Nielsen (1990), the data will be split randomly into a training set, a vali-174 dation set and a test set. The model is trained using the training data and after each 175 training iteration, the error on the validation data is computed. During training, this 176 error usually declines towards a minimum. Beyond this minimum, the error rises – 177 overlearning (or overfitting) occurs: the model fits the training data perfectly but does not generalize well. Hence, the model training is stopped when the error on 179 the validation set starts rising. A size ratio of 8:1:1 for training, validation and test sets is used. The data sets are partitioned randomly 20 times and the models are 181 trained. The models' performance will be determined using the root mean squared 182 error (RMSE) and the mean absolute error (MAE) on the test set. It is assumed that the reader is familiar with these measures.

4 Regression Results

The models are run with the parameter settings given below. Those were determined 186 experimentally on *F04* using a grid search, and carried over to the remaining data 187 sets. 188

MLP A relatively small number of 10 hidden neurons is used and the network is 189 trained until a minimum gradient of 0.001 is reached, using a learning rate of 190 0.25 and the *tangens hyperbolicus* sigmoid activation function.

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t2.2	Model/Dataset	MAE				RMSE			
t2.3		F04	F131	F131net	F330	F04	F131	F131net	F330
t2.4	MLP	0.3706	0.2468	0.2300	0.3576	0.4784	0.3278	0.3073	0.5020
t2.5	RBF	0.3838	0.2466	0.2404	0.3356	0.5031	0.3318	0.3205	0.4657
t2.6	REGTREE	0.4380	0.2823	0.2530	0.4151	0.5724	0.3886	0.3530	0.6014
t2.7	SVR	0.3446	0.2237	0.2082	0.3260	0.4508	0.3009	0.2743	0.4746
t2.8	LINREG	0.4285	0.3257	0.2766	0.3820	0.5578	0.4392	0.3871	0.5330
t2.9	NAIVE	2.9061	0.6135	0.6492	4.7157	3.1253	0.7613	0.7847	4.8308

t2.1 **Table 2** Results of running different models on different data sets. The best predictive model for each data set is marked in **bold** font

- RBF For the radial basis function network, a radius of 1 is used for the radial basis 192 neurons in the hidden layer. The algorithm, which incrementally adds neurons 193 until the error goal of 0.001 is met, uses a maximum number of 70 neurons.
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- RegTreeFor the regression tree, the default settings of classregtree perform opti-195mal; the full tree is pruned automatically and the minimum number of training196examples below which no split should be done is 10.197
- SVR For the support vector regression model, the radial basis function kernel 198 yields the best results, using the parameters C = 60, $\sigma = 4.0$ and $\xi = 0.2$. 199

Considering the results in Table 2, support vector regression obviously performs 200 best on all but one of the data sets, regarding both error measures. Furthermore, 201 SVR also is the model taking the least amount of computation time. Hence, the 202 slight difference between the RMSE of SVR and RBF on the *F330* data set may 203 be considered insignificant in practice when computational cost is also taken into 204 account when deciding for a model. Regarding the understandability of the gener-205 ated models, it would certainly be desirable to have the regression tree as the best 206 model since simple decision rules can easily be generated from the tree. However, 207 the regression tree performs worst in all of the cases. On the other hand, when comparing the hitherto reference model MLP with the current best model SVR, there is 209 not much difference in the understandability of both models. 210

5 Conclusion

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The results clearly show that support vector regression can serve as a better reference 212 model for yield prediction than MLP. Even if the improvement should be statistically 213 insignificant, the advantages of SVR over MLP remain. It is computationally less 214 demanding, at least as understandable as the MLP and, most importantly, mostly 215 produces better yield predictions. Furthermore, the comparison against a linear 216 regression baseline and a naive estimator shows that the additional effort for using 217 SVR is worth it. 218

Furthermore, the results also show that model parameters which have been estab-219 lished on one data set can be carried over to different (but similar with respect 220 to the attributes) data sets. A model for identifying the most useful heterogeneity 221 indicators is currently being evaluated. 222



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5.1 Future Work

Due to the relatively high spatial resolution of the input data, the possible issue 224 of spatial autocorrelation arises. This influences the modeling during the cross-225 validation stage. This will be investigated in future work. 226

Acknowledgements Experiments have been conducted using Matlab 2008a. The field trial data 227 came from the experimental farm Görzig of Martin-Luther-University Halle-Wittenberg, Germany. 228

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