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To cite this article: Julian Hagenauer, Hichem Omrani & Marco Helbich (2019) Assessing the performance of 38 machine learning models: the case of land consumption rates in Bavaria, Germany, International Journal of Geographical Information Science, 33:7, 1399-1419, DOI: [10.1080/13658816.2019.1579333](https://doi.org/10.1080/13658816.2019.1579333)

To link to this article: <https://doi.org/10.1080/13658816.2019.1579333>



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# Assessing the performance of 38 machine learning models: the case of land consumption rates in Bavaria, Germany

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## ABSTRACT

Machine learning (ML) is at the forefront of land-use change modeling. Due to numerous available ML approaches, the model choice is complex and usually based on ad hoc decisions, though informed through a few comparative studies that considered a limited number of models. This study contributes a comprehensive comparison of 38 ML models to examine land consumption rates (LCR) (i.e. the transition of landscapes to built-up areas). We modeled LCR for 2009–2015 in Bavaria, Germany, and predicted rates for 2015–2021 at a municipality level. To assess the performance of each approach, we measured the mean absolute error (MAE), the root-mean-square error (RMSE), and the coefficient of determination ( $R^2$ ) using cross-validation. All algorithms consistently predicted that the land consumption rate for Bavaria will increase. eXtreme gradient boosting decision trees performed best with respect to the RMSE (0.500) and  $R^2$  (0.183), while the support vector machine with polynomial kernel has the lowest MAE (0.288). The generalized additive model and the random forest models also performed well. We recommend these ML approaches for future land consumption and land-use change studies. A poor performance was found for recursive partitioning by decision trees, self-organizing maps, and partitioning using deletion, substitution, and addition moves.

## ARTICLE HISTORY

Received 17 June 2018

Accepted 3 February 2019

## KEYWORDS

Land consumption; land-use; machine learning; model comparison; Germany

## 1. Introduction

Land-use mapping and modeling of environmental data using machine learning (ML) (Witten *et al.* 2016) have gained increasing interest within the geospatial community (Lary *et al.* 2016). It has become a vital methodology to monitor (Rogan *et al.* 2008, Qian *et al.* 2014, Heung *et al.* 2016, Omrani *et al.* 2019) and forecast land-use change (Samardžić-Petrović *et al.* 2016, Shafizadeh-Moghadam *et al.* 2017, Du *et al.* 2018, Hagenauer and Helbich 2018). ML comprises a set of inductive models that recognize patterns and/or minimize the prediction error of complex regression functions, by means of a repeated learning strategy from training data, linking an output such as land-use change to several underlying drivers. Once learned, the model can then be used to estimate previously unseen cases and predict future land-use change (Brown *et al.* 2013, Tayyebi and Pijanowski 2014, Lary *et al.* 2016, Maxwell *et al.* 2018).

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 Supplemental data for this article can be accessed [here](#).

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Statistical land-use models such as ordinary least squares regression or logistic binary regression are vital to understand land-use change processes and have thus gained popularity (Veldkamp and Lambin 2001, Lambin and Geist 2008, Jokar Arsanjani *et al.* 2013, Shafizadeh-Moghadam and Helbich 2015, Mustafa *et al.* 2018). While these basic statistical models have a long tradition and have contributed to our understanding of how land-use change takes place across space and over time due to anthropogenic influences (Brown *et al.* 2004, Seto *et al.* 2012), the results are only reliable when model assumptions are fulfilled. These assumptions include that the drivers underlying land-use change are not correlated and that residuals (i.e. the difference between observed and predicted values) follow a specific distribution while being homoscedastic (i.e. having similar variance) (Fahrmeir *et al.* 2013). Of equal importance, these models are frequently restricted to linear associations (Dubovyk *et al.* 2011, Jokar Arsanjani *et al.* 2013), which seems a rather implausible assumption, as shown by a few studies (Tayyebi and Pijanowski 2014). Although non-linearity can be incorporated through polynomial terms or splines (Fahrmeir *et al.* 2013), some prior knowledge about the underlying correlations is still required, though it is rarely available. Similarly, it seems of ultimate importance to consider not only the drivers' main effects but also the interactions between them (Pijanowski *et al.* 2002). Both issues can be addressed through ML.

Data-driven models from the field of ML have recently emerged as powerful alternatives to parametric land-use models, and they hold great promise (Hagenauer and Helbich 2012, Tayyebi and Pijanowski 2014, Rienow and Goetzke 2015, Samardžić-Petrović *et al.* 2016, Omrani *et al.* 2017, 2019, Shafizadeh-Moghadam *et al.* 2017, Du *et al.* 2018). ML models have manifold benefits. For example, they are capable of dealing with massive amounts of data and a large number of variables, and they have the ability to model complex non-linear relationships as well as interactions between drivers, while not being grounded in restrictive distributional assumptions of the input data that are hard to achieve in practice (Witten *et al.* 2016).

The repertoire of ML is large (Lim *et al.* 2000, Fernández-Delgado *et al.* 2014), which makes the selection of a well-performing model a challenging task. However, frequently only a single approach is applied (Azari *et al.*, 2016, Huang *et al.* 2010, Hagenauer and Helbich 2012, Linard *et al.* 2013, Samardžić-Petrović *et al.* 2016, Omrani *et al.* 2019), often either artificial neural networks (Haykin 2009), random forests (Breiman 2001), and support vector machines (Scholkopf and Smola 2001). To support an evidence-based algorithmic selection, a small number of land-use studies have compared multiple ML algorithms (Rogan *et al.* 2008, Tayyebi and Pijanowski 2014, Samardžić-Petrović *et al.* 2017, Shafizadeh-Moghadam *et al.* 2017). While supportive, these studies assessed the performance of only a small number of algorithms. For example, Shafizadeh-Moghadam *et al.* (2017) compared six models to generate land-use transition probability maps. Multivariate adaptive regression splines and artificial neural networks were found to predict most accurately. Another study (Samardžić-Petrović *et al.* 2017) concluded that support vector machines outperform their competitors, including neural networks and logistic regression (Huang *et al.* 2010). While consensus is building that ML outperforms parametric models (e.g. regression), findings are less uniform and partly contradictory when ML models are contrasted. However, since many other ML models exist (Fernández-Delgado *et al.* 2014), more powerful and accurate approaches than the established ones might remain unacknowledged.

Previous studies formulate land-use change as a classification problem based on binary raster cells (Tayyebi and Pijanowski 2014, Samardžić-Petrović *et al.* 2017, Shafizadeh-Moghadam *et al.* 2017), however, research dealing with land-use change from a regression-based perspective is virtually not existent. A special case of land-use change, which can analytically be explored on an area level, is the proportion of land consumption per municipality. Land consumption refers to the conversion of agricultural and forestry landscapes into built-up areas (Nuissl *et al.* 2009). As land consumption proceeds and causes an irreversible anthropogenic process (e.g. a loss of biodiversity, atmospheric pollution) (Seto *et al.* 2012, Bren D'Amour *et al.* 2016), it is of importance for policymakers to have the most accurate forecasts available in order to formulate sustainable planning policies.

To address these research gaps, a comprehensive comparison of numerous models is needed to evaluate the suitability of individual regression-based models and to identify their individual strengths and weaknesses. The present study rigorously cross-compared 38 ML models based on data on land consumption data in Bavaria, Germany. Our selected algorithms included tree-based models, artificial neural networks, support vector machines, linear regression models, nearest neighbor algorithms, and rule-based learners. The selection was guided by their proliferation in other domains. Yet, to the best of our knowledge, some of them had never been tested, and such an extensive model comparison had neither been conducted in the context of modeling land-use change nor modeling land consumption. The research question was as follows: Which algorithm predicts land consumption rates most accurately, while still being computationally moderately intense?

This article is structured as follows: [Section 2](#) outlines the study area and the data; [Section 3](#) introduces the methods; [Section 4](#) summarizes the results; [Section 5](#) discusses the findings in the context of the existing literature; and [Section 6](#) draws conclusions.

## 2. Materials

### 2.1. Study area

Germany faces one of the highest rates of land consumption of all EU member states (Siedentop and Kausch 2004, Kroll and Haase 2010). The federal government of Germany aims to limit the amount of land consumption to 30 ha per day up to the year 2020 (Statistisches Bundesamt 2012). This corresponds to a land consumption rate (LCR) of 0.43% of Germany's total area in six years. For this model comparison, we selected the federal state of Bavaria, Germany, as the study area. Its approximately 12.977 million inhabitants make it the second most populated federal state in Germany, and its 70,550 km<sup>2</sup> make it the largest one. The area of Bavaria accounts for 19.47% of the total area of Germany.

### 2.2. Data

We analyzed LCR at a municipality level for 2009–2015. After removing unincorporated municipalities (e.g. Chiemsee and Veldensteiner Forst), the dataset included 2,056 municipalities.<sup>1</sup> For each municipality, the LCR for both time periods were determined by dividing the difference between the consumed land (e.g. built-up areas, transportation infrastructure) in the beginning and end of the period by the total area of the

municipality and multiplying it by 100 to obtain percentages. Data were extracted from the IÖR Monitor,<sup>2</sup> which is based on the digital landscape model ATKIS®–Basis-DLM (Meinel and Schumacher 2010).

A set of 10 demographic, socioeconomic, and environmental covariates were used as explanatory variables that were assumed to influence land-use change (Dubovyk *et al.* 2011, Kretschmer *et al.* 2015, Hagenauer and Helbich 2018). Unless stated otherwise, the data were obtained from Germany's regional database (Regionaldatenbank Deutschland),<sup>3</sup> whose tables are based on the Regional Statistical Data Catalog and the Regional Statistical special program of the Federal Statistical Office and the statistical offices of the federal states. The demographic and socioeconomic variables were collected for 2009 and 2015.

In line with urban theory (Duranton and Turner 2012), the spatial distance (in km) from each municipality to the nearest regional center (Oberzentrum) was considered to reflect that accessibility stimulates urban growth. To incorporate the wealth per municipality which was found to be associated with urban growth (Bloom *et al.* 2008), employment rate (in %) served as a proxy variable. We used the in- and out-commuter rates (in %) as indicators to adjust for urbanization pressure through the population in- and outflows. As urban and rural municipalities may be affected differently, we controlled for the degree of urbanity by means of the logged population density (in 1,000 people per km<sup>2</sup>) (Hagenauer and Helbich 2018). Data on the trade tax (in €1,000 per capita) were included to represent the municipalities' economic prosperity. Since the potential for further urban change decreases with the amount of existing built-up land, we considered the proportion of built-up area per municipality (in %). The variable was log transformed to make it Gaussian-like distributed. We included the mean of the terrain ruggedness index (Riley *et al.* 1999) to account for different building potentials due to topologic variation. Elevation data with a resolution of 90 m obtained from the Shuttle Radar Topology Mission served as the basis. Finally, the longitude and the latitude of the center of each municipality were included in order to account for the (unmeasured) locational characteristics (Jokar Arsanjani *et al.* 2013). Both longitude and latitude were scaled to zero and one, maintaining the aspect ratio. Table 1 provides descriptive statistics for all variables.

### 3. Methods

This section briefly describes each of the 38 ML models and their tunable parameters. All models have either already been used in land-use research or have shown promising results in other model comparisons (Fernández-Delgado *et al.* 2014, Xu *et al.* 2014).

All analysis steps were performed in the *R* programming environment (R Core Team 2018) using the caret package (Kuhn 2008). The latter is particularly useful for model comparisons as it harmonizes and streamlines the workflow for predictive models, parameter tuning, and validation, while providing a unified interface for each algorithm. A list of the tested models together with a short description is presented in Table 2. Note that the tested parameter values are given in the notation A:B:C, referring to the integer values A to B with a step size C. We also extended the default values of the tunable parameter values of caret to provide more comprehensive parameter tuning. The *R* code is provided as supplementary materials.

Before the ML models were built, not available values (NAs) were imputed using a bagging ensemble of trees (Feelders 1999). The input variables were then scaled to

**Table 1.** Descriptive statistics for the response and the covariates for 2009 and 2015.

Response variable	Min.	1st quartile	Median	Mean	3rd quartile	Max.	NAs
Land consumption rate for 2009–2015	−5.200	0.300	0.500	0.611	0.800	5.500	0
Covariates 2009							
Distance to regional center	0.000	8.780	15.600	16.800	23.800	54.400	0
In-commuter rate	0.238	0.611	0.685	0.682	0.759	0.952	27
Latitude	0.000	0.272	0.480	0.499	0.741	1.000	0
Longitude	0.000	0.298	0.447	0.464	0.627	0.980	0
Out-commuter rate	0.255	0.781	0.873	0.828	0.917	0.988	0
Population density (log)	0.766	1.830	2.000	2.080	2.260	3.630	0
Proportion of built-up area (log)	0.000	0.778	0.875	0.920	1.030	1.920	0
Terrain ruggedness (log)	2.938	11.931	15.896	18.525	21.567	112.918	0
Trade tax	−1.320	0.082	0.149	0.254	0.280	19.500	0
Unemployment rate	0.003	0.014	0.018	0.019	0.023	0.048	0
Covariates 2015							
Distance to regional center	0.000	8.780	15.600	16.800	23.800	54.400	0
In-commuter rate	0.228	0.634	0.702	0.701	0.774	0.964	22
Latitude	0.000	0.272	0.480	0.499	0.741	1.000	0
Longitude	0.000	0.298	0.447	0.464	0.627	0.980	0
Out-commuter rate	0.230	0.790	0.875	0.834	0.918	0.993	0
Population density (log)	0.817	1.830	2.010	2.080	2.270	3.670	0
Proportion of built-up area (log)	0.079	0.806	0.908	0.950	1.060	1.910	0
Terrain ruggedness (log)	2.938	11.931	15.896	18.525	21.567	112.918	0
Trade tax	−0.026	0.147	0.246	0.380	0.413	16.500	0
Unemployment rate	0.002	0.011	0.014	0.015	0.017	0.040	0

have zero mean and unit variance in order to make them comparable. The out-of-sample performance of the models (i.e. MAE, RMSE, and  $R^2$ ) with selected parameters was evaluated through 10-fold cross-validation (Kuhn 2008). This procedure randomly partitions the data into 10 disjoint subsets. One subset at a time is then used for testing the model, while the remaining sets are used to build the model. This reduces the bias in performance estimation since the testing and training data sets are independent of each other (Kohavi 1995). Cross-validation was repeated four times to lower the variance of the estimated performance and the results were averaged. We used the covariates of 2009 to perform cross-validation and determine the best parameters. Then, using the best parameters, the final model was built using the same data. Finally, the covariates of 2015 were applied to the model to predict LCRs for 2015–2021. Figure 1 summarizes the workflow.

To evaluate the different classifiers, the distribution of the performance statistics needed to be taken into account (Hothorn *et al.* 2005). We evaluated the statistical significance of the models' differences in performance as follows: Kruskal–Wallis tests with a 5% significance level were employed to test the null hypothesis that the performance estimates of the models are not systematically different from each other. Two-sided Wilcoxon rank-sum tests were applied to determine the statistical significance of systematic pairwise differences between models. To control for a false discovery rate at the 5% level, the  $p$ -values were adjusted by means of the Benjamini–Hochberg procedure (Benjamini and Hochberg 1995).

## 4. Results

Figure 2 summarizes the performance of the classifiers. The lowest mean MAE was achieved by *svmPoly* (0.288), while *xgbTree* had the highest mean  $R^2$  (0.183) and the lowest mean RMSE (0.500). However, the differences between *xgbTree* and *svmPoly* in

**Table 2.** Summary of the tested models.

Label	Description	R package	Tested parameters	References	Model class
<i>brnn</i>	Bayesian regularized neural network	brnn	neurons = $2^{(0.5:1)}$	(Dan Foresee and Hagan 1997; Mackay 1992)	NN
<i>cforest</i>	Random forest using conditional inference trees	party	mtry = 1:10:1	(Strobl <i>et al.</i> 2008)	Bag, Tree
<i>ctree</i> <i>cubist</i>	Conditional decision tree Rule-based model that extends Quinlan's M5 model tree	party cubist	mincriterion = 0.8:0.99:0.01 committees = 1:10:1; neighbors = 0:9:1	(Hothorn <i>et al.</i> 2006) (Quinlan 1993a, 1993b, 1992)	Tree Boost,
Tree, LM					
<i>earth</i> <i>elm</i>	Multivariate adaptive regression splines Extreme learning machine	earth elmNN	Degree = 1:4:1; nprune = $2^{(0.5:1)}$ actfun = radbas, sind, purelin, tansig; nhid = $2^{(0.5:1)}$	(Friedman 1991) (Guang-Bin Huang <i>et al.</i> 2012)	Spline NN
<i>enet</i> <i>gam</i>	Elastic Net Generalized additive model	elasticnet mgcv	fraction = 0:1:0.05; lambda = $10^{(-6:-1:1)}$ select = True,False; method = GCV,Cp	(Zou and Hastie 2005) (Hastie and Tibshirani 1986)	LM Add
<i>gbm</i>	Generalized boosting regression machine	gbm	n.trees = 500; interaction.depth = 4:16:4, shrinkage = 0.01, 0.02, 0.05; n.minobsnode = 4:32:4 degree = 1:3:1	(Friedman 2001)	Boost, Tree
<i>gcvEarth</i> <i>glm</i>	Earth using generalized cross-validation Generalized linear model	earth stats		(Friedman 1991) (McCullagh and Nelder 1998)	Spline LM
<i>glmnet</i>	Generalized linear model using penalized maximum likelihood with L1 and/or L2 regularization		alpha = 0:1:0.05; lambda = $10^{(-6:-1:1)}$	(Friedman <i>et al.</i> 2010; Simon <i>et al.</i> 2011)	LM
<i>kknn</i>	Weighted sum of k nearest neighbors	kknn	kernel = gaussian, optimal, rank, inv; k = 10:90:2; distance = c	(Hechenbichler and Schliep 2004; Samworth 2012)	Avg
<i>knn</i> <i>lars</i> <i>lasso</i> <i>monmlp</i>	Average of k nearest neighbors Least angle regression Linear regression with L1 regularization Ensemble of neural networks with monotonic constraints	class lars elasticnet monmlp	k = 1:100:1 fraction = 0:1:0.05 fraction = 0:1:0.05 hidden1 = $2^{(0.5:1)}$ ; n.ensemble = 1:4:1	(Efron <i>et al.</i> 2004) (Zou and Hastie 2005) (Lang 2005; Zhang and Zhang 1999)	Avg LM LM Bag, NN
<i>nnet</i> <i>partDSA</i>	Neural network Piecewise constant estimation sieve of candidate estimators based on a comprehensive search over the covariate space	nnet partDSA	size = $2^{(0.5:1)}$ ; decay = $10^{(-6:-1:1)}$ cut.off.growth = 1:10:1;MPD = 0.1:1:0.1	(Haykin 2004) (Molinaro <i>et al.</i> 2010)	NN Tree

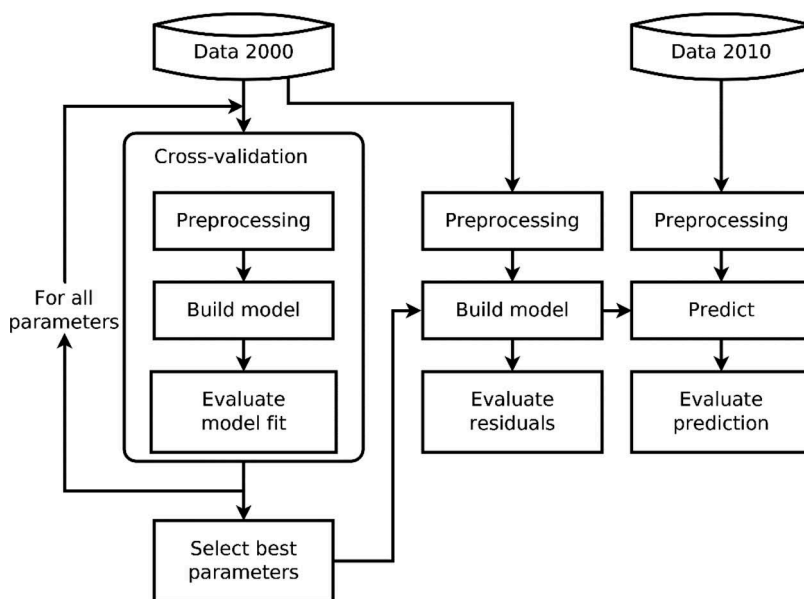
(Continued)

Table 2. (Continued).

Label	Description	R package	Tested parameters	References	Model class
<i>pcaNet</i>	Neural network with principal component preprocessing	nnet	size = 2 <sup>(0.5:1)</sup> ; decay = 10 <sup>(-6:-1:1)</sup>	(Eleyan and Demirel 2005)	NN
<i>pcr</i>	Principal component regression	pls	n.comp = 1:9:1	(Jolliffe 1982)	LM
<i>penalized</i>	Generalized linear model with L1 and/or L2 regularization	penalized		(Goeman 2010)	LM
<i>pls</i>	Partial least squares regression	pls	ncomp = 1:4:1, 8	(Wold et al. 1984)	LM
<i>ppr</i>	Projection pursuit regression	ppr	nterms = 1:9:1	(Friedman and Stuetzle 1981)	Add
<i>ranger</i>	Random forest	ranger	mtry = 1:10:1; min.obs.size = 5; splitrule = variance, extratrees	(Wright and Ziegler 2017)	Bag, Tree
<i>rf</i>	Random forest	randomForest	mtry = 1:10:1	(Breiman 2001)	Bag, Tree
<i>ridge</i>	Linear regression with L2 regularization	elasticnet	lambda = 0:1:0.05	(Zou and Hastie 2005)	LM
<i>rlm</i>	Robust linear regression that uses Huber's M-estimators	MASS	intercept = True; False; psi = humber, hampel, bisquare	(Huber 1981)	LM
<i>rpart</i>	Decision tree	rpart	complexity = 0.001:0.1:0.001	(Breiman et al. 1984)	Tree
<i>rqnc</i>	Non-convex penalized quantile regression	rqpen	penalty = SCAD, MCP; lambda = 10 <sup>(-6:-1:1)</sup>	(Fan and Li 2001; Tibshirani 1996)	LM
<i>spikeslab</i>	Spike and slab model using a continuous bimodal prior	spikeslab	var = 1:9:1	(Ishwaran et al. 2010)	LM
<i>spls</i>	Sparse partial least squares regression	spls	k = 1:9:1; kappa = 0:05:01; eta = 0:1:0.005	(Chun and Keleş 2010)	LM
<i>svmLinear</i>	Support vector machine with linear kernel	kernlab	C = 0.05:1:0.05	(Cortes and Vapnik 1995; Drucker et al. 1997)	SVM
<i>svmPoly</i>	Support vector machine with polynomial kernel	kernlab	degree = 1:3:1; scale = 0.01, 0.05, 0.1, 0.2; C = 0.1:1:0.1	(Cortes and Vapnik 1995; Drucker et al. 1997)	SVM
<i>svmRadial</i>	Support vector machine with radial basis kernel	kernlab	C = 0.1:1:0.1; sigma = 0.01, 0.02, 0.05, 0.1, 0.15, 0.2	(Cortes and Vapnik 1995; Drucker et al. 1997)	SVM
<i>treebag</i>	Bagging ensemble of decision trees	ipred		(Breiman 1996; Hothorn and Lausen 2005)	Bag, Tree
<i>xgbTree</i>	eXtreme gradient boosting decision trees	xgboost	eta = 0.02; gamma = 0; nrounds = 500; max_depth = 8:24:4, colsample_bytree = 0.3:0.7:0.2; subsample = 0.8:1.0:0.1, min_child_weight = 0.8:1.0:0.1	(Chen and Guestrin 2016)	Boost, Tree
<i>xyf</i>	Self-organizing map	kohonen	topo = hexagonal; xdim = 1,2,4,6,8,12; ydim = 1,2,4,6,8,12; user.weights = 0.2:0.8:0.2	(Kohonen 2001)	Avg

LM = linear model, NN = neural network, Avg = local averaging, SVM = support vector machine, Tree = decision tree, Bag = bagging, Boost = bootstrap aggregating, Add = additive model, Spline = model using splines.





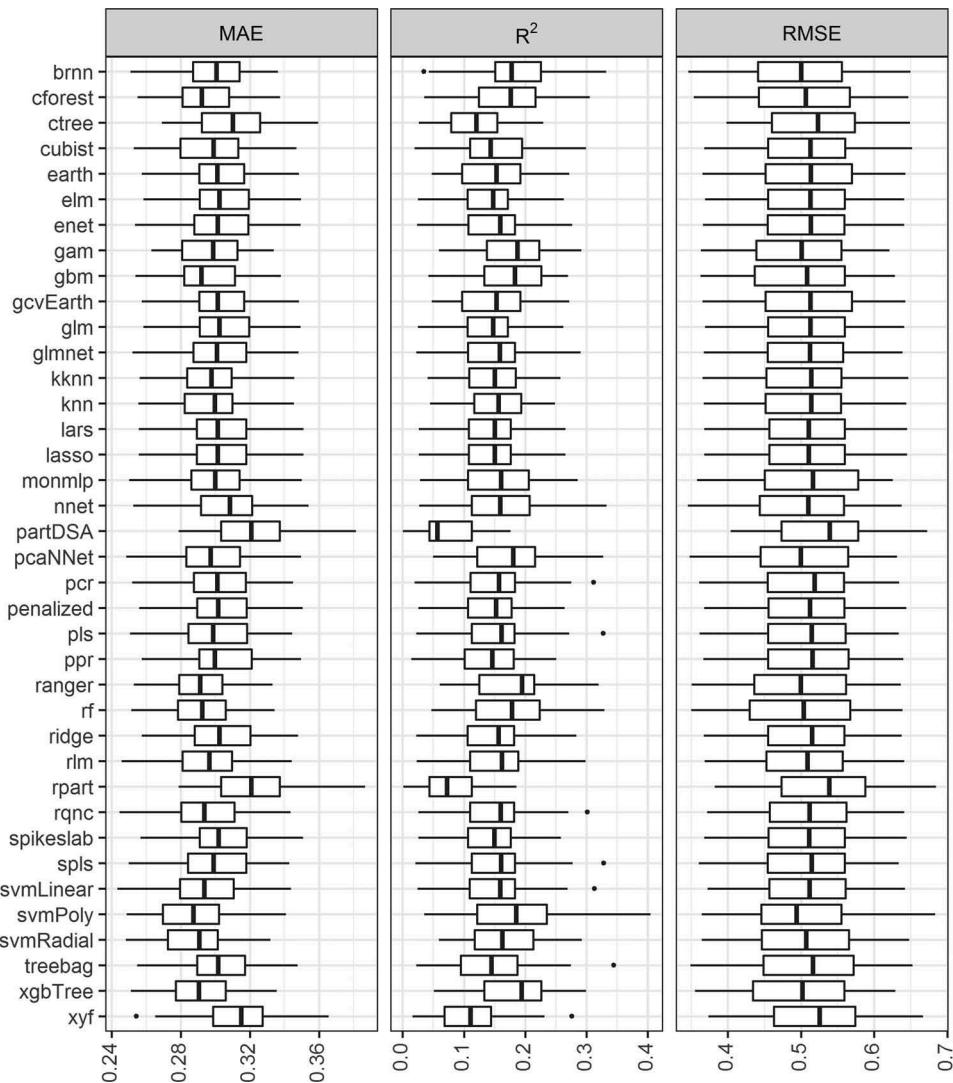
**Figure 1.** Workflow of parameter selection, model building, and prediction.

mean MAE were minor. The *partDSA* model generally achieved the lowest performance; its mean RMSE (0.535) and mean MAE (0.321) were higher and its mean  $R^2$  (0.075) was lower than any other model.

The null hypothesis of no performance differences between the classifiers was rejected by the Kruskal–Wallis test at 5% significance level for MAE and  $R^2$  but not for RMSE ( $p < 0.05$ ). The null hypothesis of the Wilcoxon rank-sum of equal medians was rejected for many pairs of models for MAE and RMSE ( $p < 0.05$ ); for RMSE, the null hypothesis was not rejected for any pair of models. With respect to RMSE and  $R^2$ , the null hypothesis of equal medians was not rejected for any pair of *gam*, *svmRadial*, and the tree-based ensemble models *rf*, *xgbTree*, *ranger*, *gbm*, and *cforest*. However, the null hypothesis was mostly rejected when comparing these models with linear models (e.g. *glm*, *lasso*, and *ridge*) or single tree models (e.g. *rpart* and *ctree*), indicating significant performance differences. Detailed results are given in the supplementary materials (Table S1–S3).

As an example, [Figure 3](#) depicts the residuals of the *xgbTree* model (left panel), which is among the best performing models and, for comparison purposes, the residuals of *nnet* (right panel). While in general the residual means were similar across the study area, some minor patterns were observable. For instance, the figure shows *xgbTree* and *nnet* both underestimate the LCR for the city of Straubing and its surroundings (a), while they overestimate the LCR for the city of Augsburg and its surroundings (b). However, despite the overall better performance of *xgbTree* ([Figure 2](#)), it underestimates the LCR for region (a) more than *nnet*. Furthermore, *xgbTree* underestimates and *nnet* overestimates the LCR for the municipality of Hof (c).

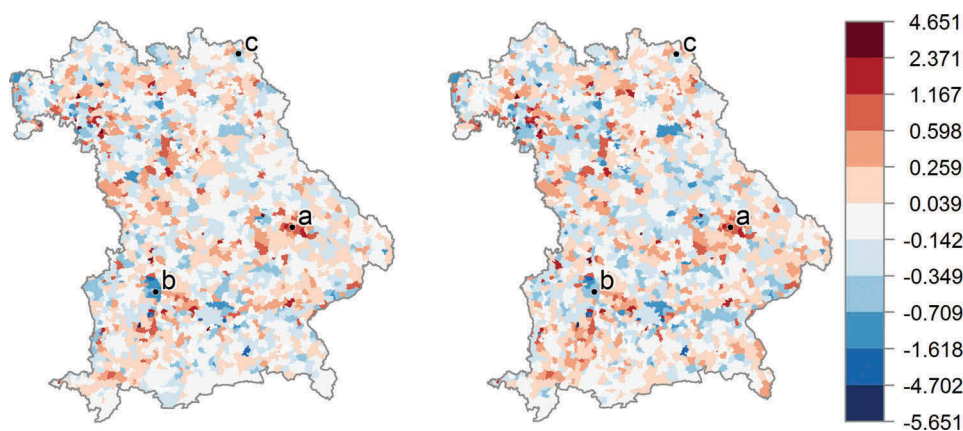
[Figure 4](#) shows the predicted mean LCRs for 2015–2021 in percentage (left panel) and the absolute LCR for the same period in ha per day (right panel). The latter refers to an



**Figure 2.** Performance boxplots calculated from the cross-validation results.

absolute measure that takes the municipality's area into account. The lowest mean LCR and absolute LCR were predicted by *cubist* (0.580% and 16.924 ha per day). The highest mean LCR was predicted by *ridge* (0.646%), while the highest absolute LCR was predicted by *rpart* (19.056 ha per day).

For 2009–2015, the observed mean LCR for Bavaria was 0.611%, which corresponds to an absolute LCR of 17.444 ha per day. For 2015–2021, almost all models predicted an increase in mean LCR and absolute LCR compared to 2009–2015. Since Bavaria is the federal state of Germany with the largest area, this result seriously challenges the German policy goal to limit LCR to 30 ha per day until 2020 (Statistisches Bundesamt 2012). The few models that predicted a decrease in both measures were *cubist*, *rqnc*, and



**Figure 3.** Residuals of the *xgbTree* model (left) and *nnet* model (right).

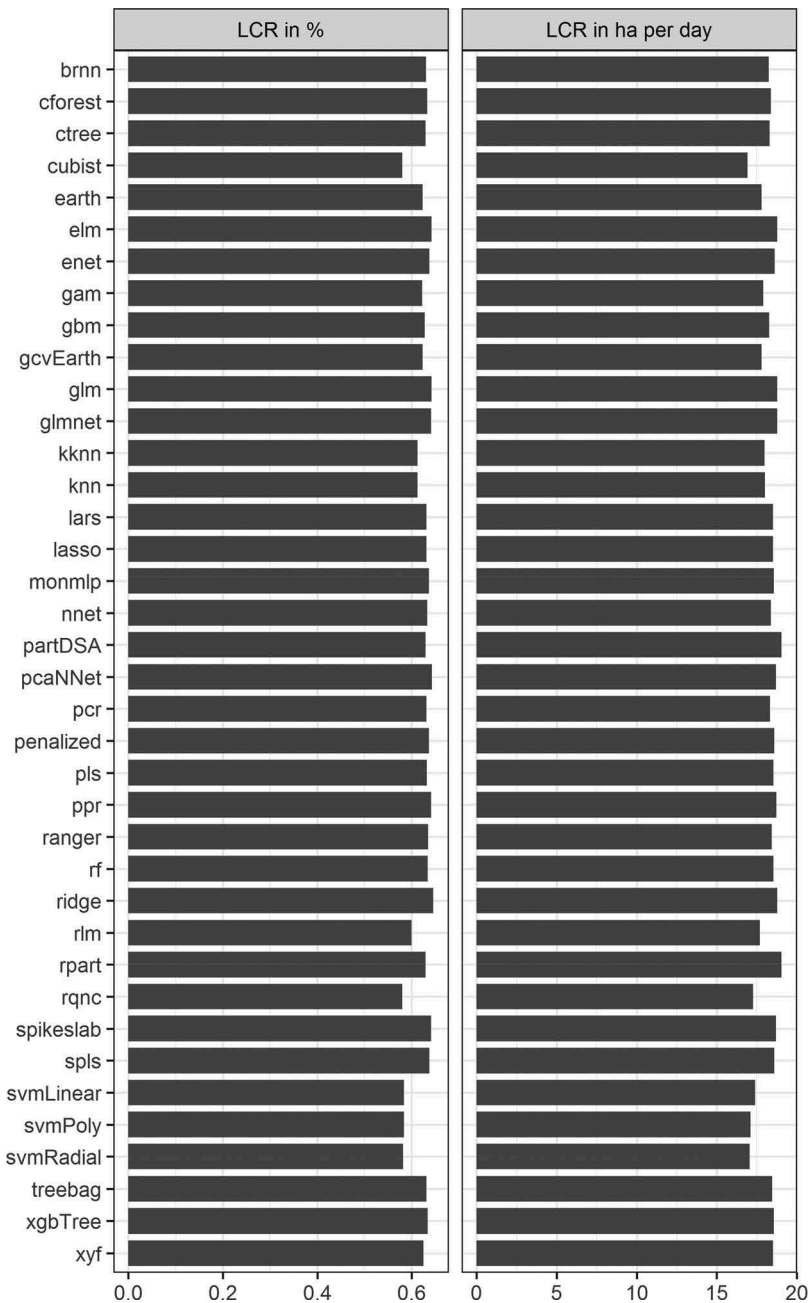
*svmLinear*, *svmRadial*, and *svmPoly*. A decrease in mean LCR and an increase in absolute LCR was predicted only by *rlm*.

**Figure 5** compares the observed LCR for 2009–2015 (i.e. the response variable, left panel) and the predicted LCRs for 2015–2021 based on the *xgbTree* model (right panel). The model predicted for most municipalities an increase in LCR. A decrease in LCR was predicted for Straubing (a) and Nuremberg (c) and their vicinities, while a substantial increase was predicted for Augsburg (b) and its vicinity. Moreover, it can be seen that Augsburg's increase in LCR is much higher than that of Munich (d).

To show the influence of the different covariates on LCR, the importance of the variables for the *xgbTree* model is shown in **Figure 6**. Gain refers to the improvement in performance that is brought by a variable to the branches it is on. Cover measures the relative number of observations related to a variable. Frequency is the proportion of how many times a variable decides on a split in the trees. The figure shows that the present amount of built-up area, population density, and terrain ruggedness are the most important variables, while the least important are employment rate and trade tax. Latitude seems to be more important than longitude.

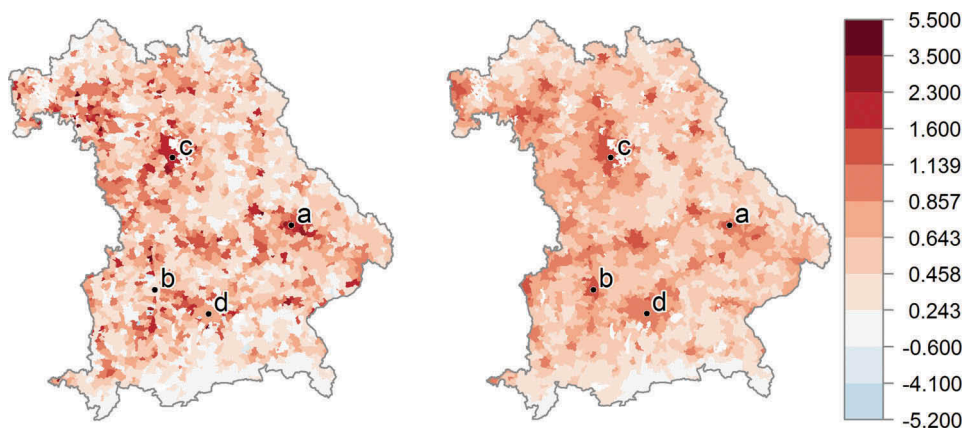
**Figure 7** shows one-way partial dependence plots (Friedman 2001) for the four most relevant variables and a joint partial dependence plot for longitude and latitude (lower panel). Partial dependence plots visualize the change in the average predicted value as one or more variables vary over their marginal distribution (Goldstein *et al.* 2015). While all variables show a non-linear association with LCR, the strength of the association varies. The LCR increases with commuter rates substantially only from values higher than 0.85. Similarly, population density shows a positive association with LCR for values lower 2.0. While the LCR increases substantially with the proportion of built-up area, in particular from values 1.0 onwards, the LCR decreases marginally with terrain ruggedness. The LCR of municipalities close to the east of Upper Palatine (a) is associated with a lower LCR than municipalities that are far apart, in particular in the far south and north-west.

Finally, **Figure 8** compares the required time to build the final models. All computations were performed on a standard laptop PC equipped with 32 GB of RAM and an

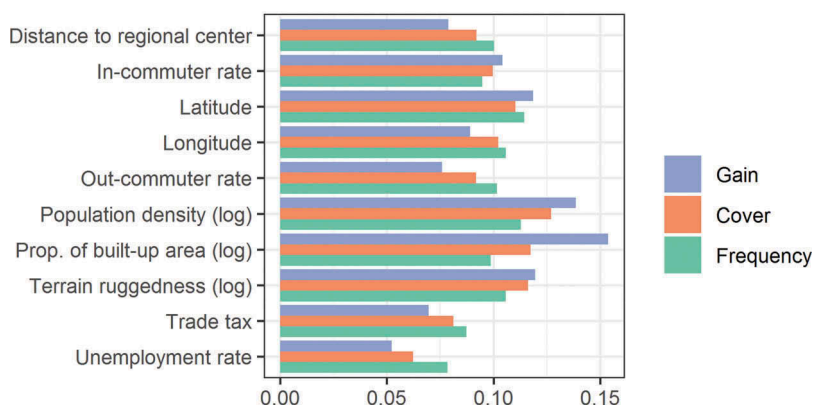


**Figure 4.** Predicted mean LCRs for 2015–2021 in percentage (left) and absolute LCR for 2015–2021 in ha per day (right).

Intel Core i7-6820HQ CPU @ 2.7 GHz. The most computational intensive was *cforest*, while the *rqnc* model was the fastest. As expected, ensemble models (e.g. *rf*, *treeBag*, *xgbTree*, *monmlp*) and support vector machine models generally took longer to build, while models based on linear regression were far less computationally intensive.



**Figure 5.** Observed LCRs for 2009–2015 (left) and predicted LCRs for 2015–2021 using *xgbTree* (right).



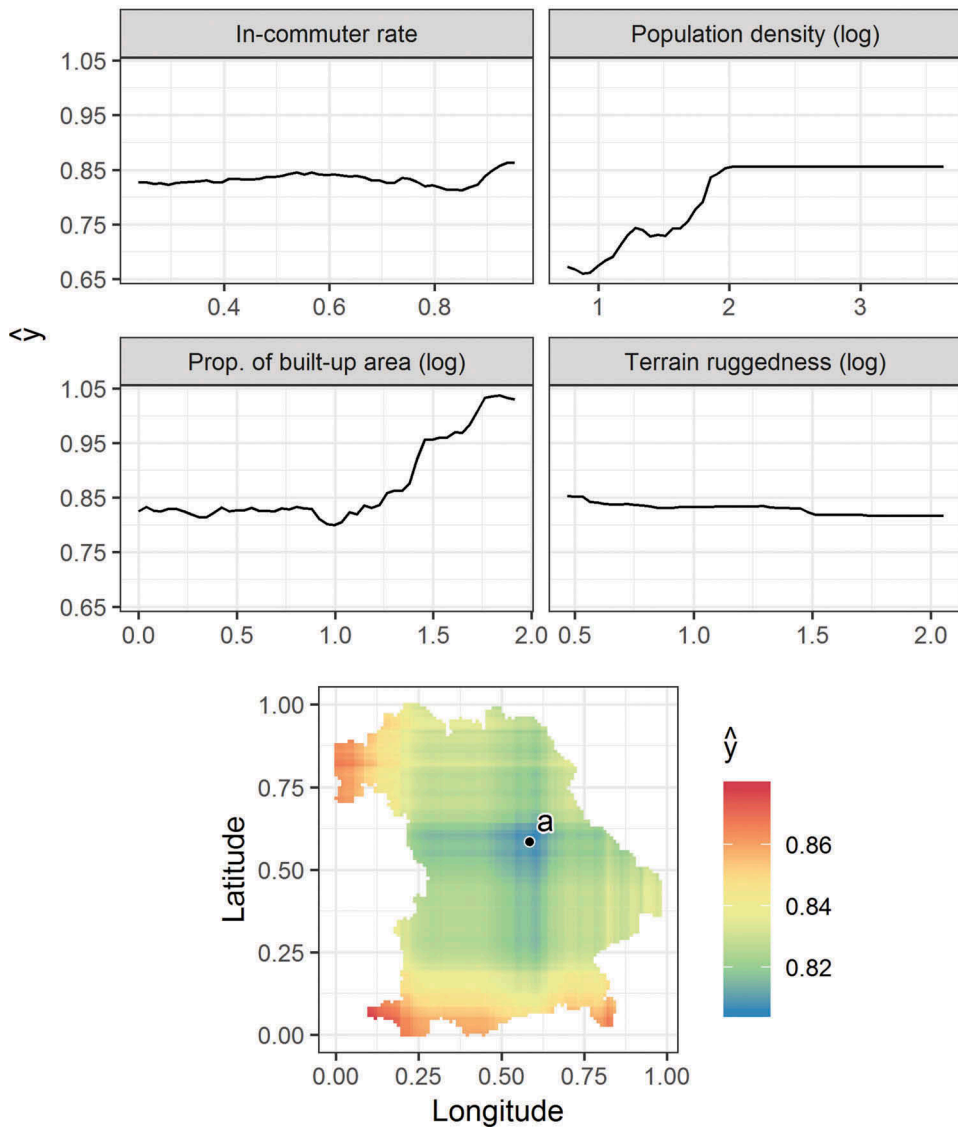
**Figure 6.** Variable importance for *xgbTree*.

Among the boosting models, running *cubist* took less time than *gbm* or *xgbTree*. In addition, *ranger* was much faster than other random forest models, such as *rf* and *cforest*.

## 5. Discussion

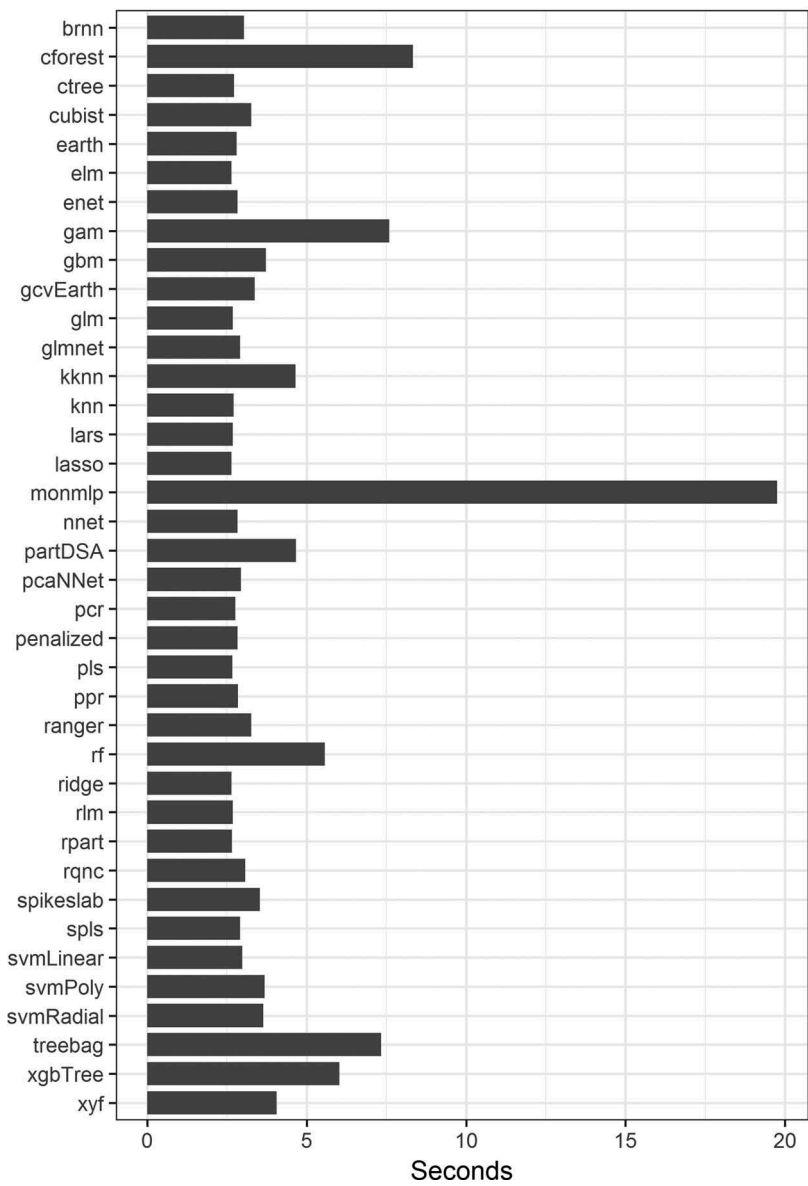
Rapid progress in ML has resulted in numerous models, necessitating comparative studies to guide application-oriented research (Fernández-Delgado *et al.* 2014). This is particularly true for land-use change science. The present study has contributed, to the best of our knowledge, the most comprehensive comparison of regression-based ML algorithms for a continuous outcome variable, namely LCR.

Generally speaking, ML has performed well in several situations, including land-use modeling where the input data is usually multidimensional (Shafizadeh-Moghadam *et al.* 2017). Our findings confirm this conclusion by indicating that *xgbTree*, *gbm*, and *gam* achieved the highest predictive accuracy compared to the other 35 models. Although



**Figure 7.** Partial dependence plots for the most relevant variables.

the *treeBag* algorithm is also a tree-based ensemble learner, it did substantially worse. We assume that this can be attributed to the tendency of *treeBag* to create correlated trees, which increases the upper bound for the generalization error (Breiman 2001). An ensemble model performs better if there is significant diversity among the sub-models forming the ensemble (Kuncheva and Whitaker 2003). Further, it is remarkable that *knn*, arguably one of the simplest models considered, performed well: It out-performed both single-tree models (e.g. *ctree* and *rpart*) and linear models (e.g. *lasso* and *glm*). This could imply that covariate interactions were minor, because, in contrast to *rpart*, *knn* is not able to model interactions among variables. This hypothesis is also supported by the very good performance of *gam*, which also does not model interactions.



**Figure 8.** Computational times to build the final models.

As we are not aware of a study similar to ours using LCR as an outcome, we discuss our findings in the general context of land-use modeling (Tayyebi and Pijanowski 2014, Samardžić-Petrović *et al.* 2017, Shafizadeh-Moghadam *et al.* 2017, Du *et al.* 2018). While existing model comparisons consider rather similar models (i.e. artificial neural networks, multivariate adaptive regression splines, classification and regression trees), the literature is inconclusive about the performance of ML algorithms, although it does acknowledge that logit regressions (Jokar Arsanjani *et al.* 2013) are out-performed by ML (Shafizadeh-Moghadam *et al.* 2017). This is in line with our findings that generalized linear models had



a weak predictive performance. The results were less clear when comparing different ML algorithms. For example, others (Tayyebi and Pijanowski 2014) report that an artificial neural network provided higher accuracy, given limited model insights, than tree-based models and multivariate adaptive regression splines. Focusing on tree-based learners, Du *et al.* (2018) found that artificial neural networks are less suited and that extremely randomized trees perform best. In our case, artificial neural networks also had only an average accuracy. Confirming previous studies (Samardžić-Petrović *et al.* 2017), we also found that support vector machines (i.e. *svmRadial*) perform better than decision trees and artificial neural networks, though our study indicates that ensemble and boosting models can achieve better results. In another multi-label classification study (Omrani *et al.* 2015), *knn* was also found to be promising.

In total, no particular model in the reviewed ML studies stands out. Moreover, none of the studies made an effort to consider spatial autocorrelation (i.e. the fact that adjacent units are more similar than distant ones (Anselin 2010)), as is done in econometric-based land-use models (Shafizadeh-Moghadam and Helbich 2015, Ay *et al.* 2016, Hagenauer and Helbich 2018). By considering the longitude and latitude per area, we attempted to adjust for unexplained locational effects. Research should prioritize exploring the impact of autocorrelation on ML models.

### 5.1. Strengths and limitations

Only a limited number of land-use studies have compared ML models, and a large majority of previous studies considered land-use change as a classification problem and used raster data as input (Shafizadeh-Moghadam *et al.* 2017). We have extended this body of knowledge towards regression-based approaches by means of modeling changes in land consumption. Another strength is that the set of tested algorithms (38 models) is significantly larger compared to available land-use change studies. This supports future ML-based studies in selecting a model that will potentially have a high predictive accuracy. Further, the models were challenged through a unified framework using optimized tuning parameters and repeating cross-validation to adjust for sampling fluctuations coupled with several goodness-of-fit metrics. In contrast to others (Du *et al.* 2018), we also compared the algorithms in terms of their computation time. We used not only distance-based variables, which are without doubt essential drivers, but also demographic, socioeconomic, and environmental variables. Finally, we used data available to the public and share the used code to ensure the reproducibility of our findings.

Despite these strengths, the following limitations need to be acknowledged. Most of these ML models use several parameters, which influences their performance. To circumvent subjective parameter selections beyond the default values, we systematically investigated values from a manually specified subspace. A more exhaustive parameter search is computationally expensive. Though done with care, we cannot entirely rule out that the optimal parameters are covered within the considered search space. As our focus relied on land consumption, an infrequently used but highly relevant outcome variable for spatial planning, it remains unclear how generalizable our results are for other land-use change outcomes. Further, data for all German municipalities were not available to us and we cannot rule out that other relevant explanatory variables were missing. Different study areas as well as diverse input data may have an impact on the model performance. We



caution against blindly using a single algorithm; instead, we recommend testing at least a few of the ones that perform well. Despite this restriction, our results provide applied land scientists with essential insights into ML model performance. To address this restriction, we advise developing a benchmark data to support future model assessments. Because we used municipality-level data, we cannot rule out that the aggregation to municipalities affected the results (Openshaw and Taylor 1979). Moreover, although our study grounds on the smallest territorial level for which data were available, the size of the tested data is moderate, as is the complexity through the number of considered covariates. Future studies should consider higher dimensional input data.

## 6. Conclusion

The selection of ML algorithms is not a straightforward task due to the large number of available alternatives. The present study performed a systematic and comprehensive comparison of 38 regression-based ML algorithms for modeling land consumption, using a variety of performance measures grounded on repeated 10-fold cross-validation.

While the ranking of the models depended to a minor extent on the consulted goodness-of-fit metrics when assessing land consumption data, our results showed that eXtreme gradient boosting decision trees (*xgbTree*) performed substantially better with respect to the RMSE (0.500) and  $R^2$  (0.183), while the support vector machine with radial basis kernel (*svmPoly*) had the lowest MAE (0.288). Of similar importance, other frequently applied ML models in land-use science only performed either moderately (e.g. *earth*, *nnet*, and *glm*) or poorly (e.g. *rpart* and *xyf*). Rarely used models such as partitioning using deletion, substitution, and addition moves (*partDSA*) and *rpart* did not perform well, independent of the performance measure. Due to their outstanding predictive performance, *xgbTree*, *gam*, and random forest models like *ranger* and *rf* seem to be a good initial choice when conducting a case study. However, we also suspect that they will not outperform the other models in all situations, and advise evaluating at least a few alternative models. Though not yet used, these well-performing ML approaches should play a major role in future land consumption and land-use studies to explore under which conditions they perform well and what results in a limited performance.

## Notes

1. <https://opendata.bayern.de/detailansicht/datensatz/verwaltungsgebiete> .
2. <https://monitor.ioer.de> .
3. <https://www.regionalstatistik.de> .

## Acknowledgments

We thank the anonymous reviewers for their constructive comments that greatly improved the article.

## Disclosure statement

No potential conflict of interest was reported by the authors.

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