Performance evaluation and hyperparameter tuning of statistical and machine-learning models using spatial data

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Outline

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3. Methods
4. Results
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Introduction

Introduction

LIFE Healthy Forest

Early detection and advanced management systems to reduce forest decline by invasive and pathogenic agents.

Main task: Spatial (modeling) analysis to support the early detection of various pathogens and prediction to other areas.

Pathogens

- Fusarium circinatum
- **Diplodia pinea** (➔ needle blight)
- Armillaria root disease
- Heterobasidion annosum

Fig. 1: Needle blight caused by **Diplodia pinea**

Motivation

- Find the model with the **highest predictive performance** for our data set.
- Results are assumed to be representative for data sets with similar predictors and different pathogens as response.
- Be aware of **spatial autocorrelation** ⚠
- Conduct "optimal" hyperparameter tuning for machine-learning models.
- Show and analyze differences in performances between spatial cross-validation and non-spatial cross-validation.

Data & Study Area

Data & Study Area

```
## Skim summary statistics
##  n obs: 926
##  n variables: 12
##
## Variable type: factor
##
## variable    missing   n     n_unique   top_counts
## ----------  --------  ----  ---------  ------------------------------------------
## diplo01     0         926   2          0: 703, 1: 223, NA: 0
## lithology   0         926   5          clas: 602, chem: 143, biol: 136, surf: 32
## soil        0         926   7          soil: 672, soil: 151, soil: 35, pron: 22
## year        0         926   4          2009: 401, 2010: 261, 2012: 162, 2011: 102
##
## Variable type: numeric
##
## variable        missing   n     mean       p0      median   p100     hist
## --------------  --------  ----  ---------  ------  -------  -------  ---------
## age             0         926   18.94      2       20       40
## elevation       0         926   338.74     0.58    327.22   885.91
## hail_prob       0         926   0.45       0.018   0.55     1
## ph              0         926   4.63       3.97    4.6      6.02
## p_sum           0         926   234.17     124.4   224.55   496.6
## r_sum           0         926   -0.00004   -0.1    0.0086   0.082
## slope_degrees   0         926   19.81      0.17    19.47    55.11
## temp            0         926   15.13      12.59   15.23    16.8
```

Data & Study Area

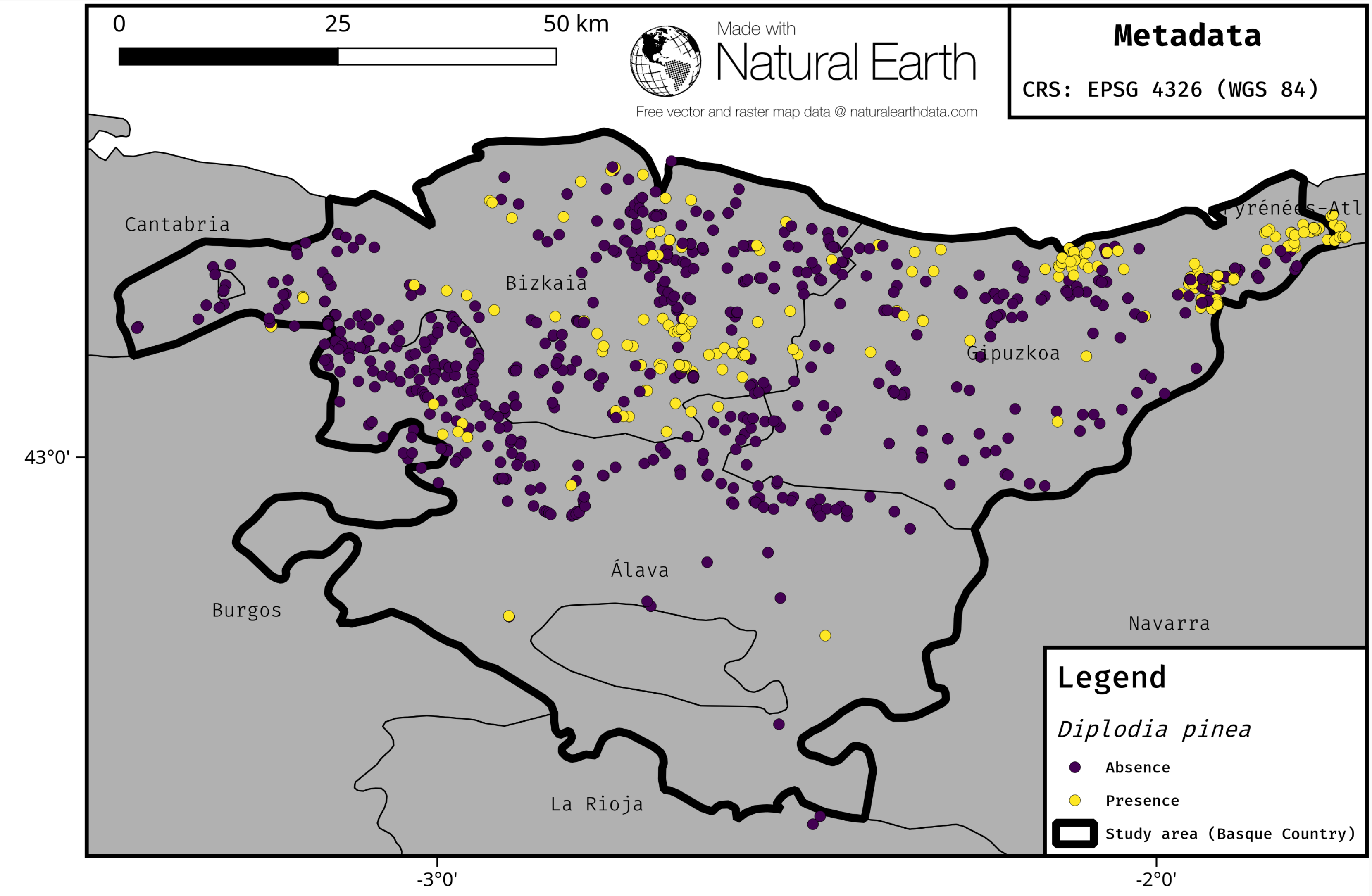

Fig. 2: Study area (Basque Country, Spain)

Methods

Methods

Machine-learning models

- Boosted Regression Trees (`BRT`)
- Random Forest (`RF`)
- Support Vector Machine (`SVM`)
- Weighted k-nearest Neighbor (`WKNN`)

Parametric models

- Generelized Addtitive Model (`GAM`)
- Generalized Linear Model (`GLM`)

Performance Measure

Area under the Receiver Operating Curve (AUROC)

Nested Cross-Validation

- Cross-validation for **performance estimation** *[outer level]*
- Cross-validation for **hyperparameter tuning** (random search) *[inner level]*

Different sampling strategies (Performance estimation/Tuning):

- Non-Spatial/Non-Spatial
- Spatial/Non-Spatial
- Spatial/Spatial
- Non-Spatial/No Tuning
- Spatial/No Tuning

Methods

Nested (spatial) Cross-Validation

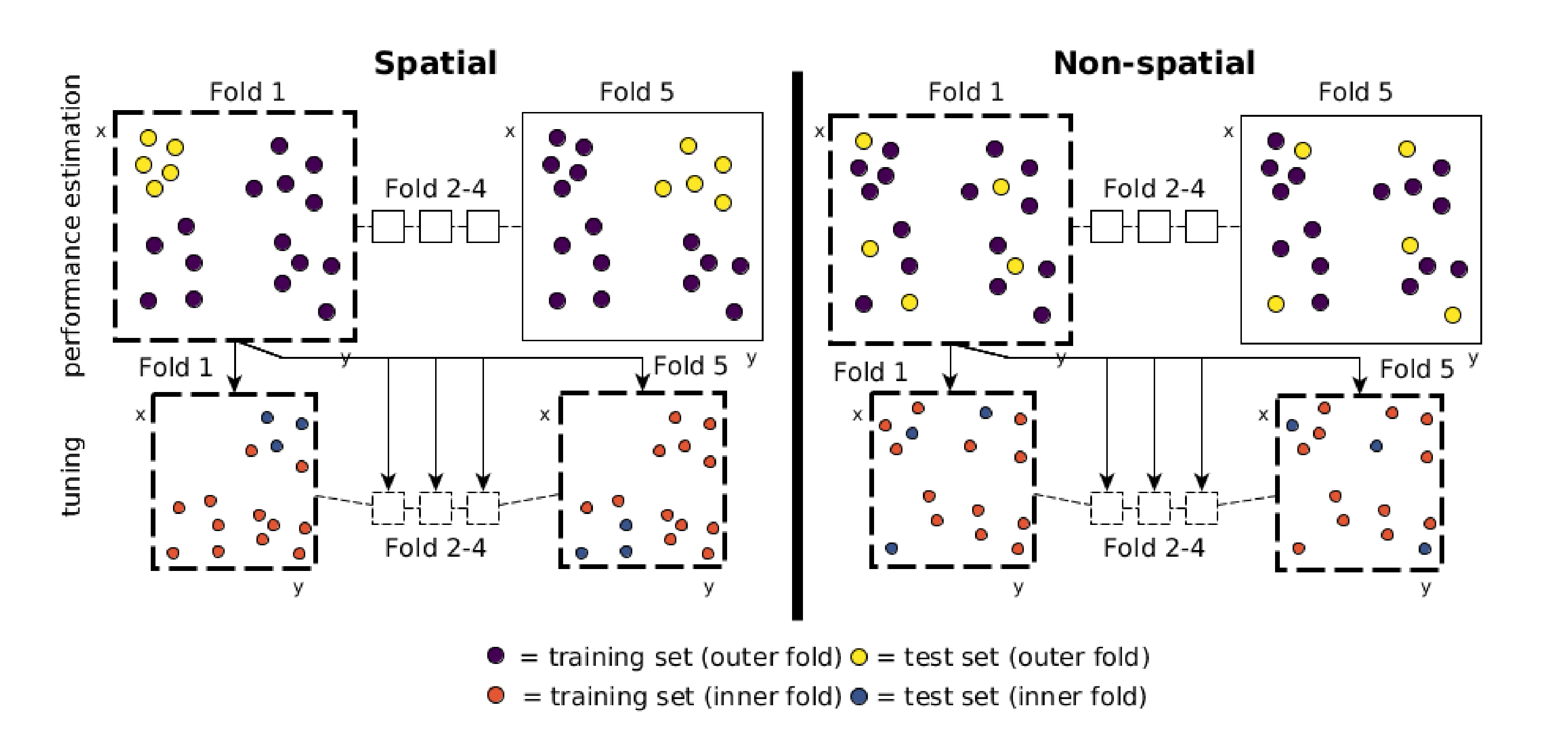

Fig. 3: Nested spatial/non-spatial cross-validation

Methods

Nested (spatial) Cross-Validation

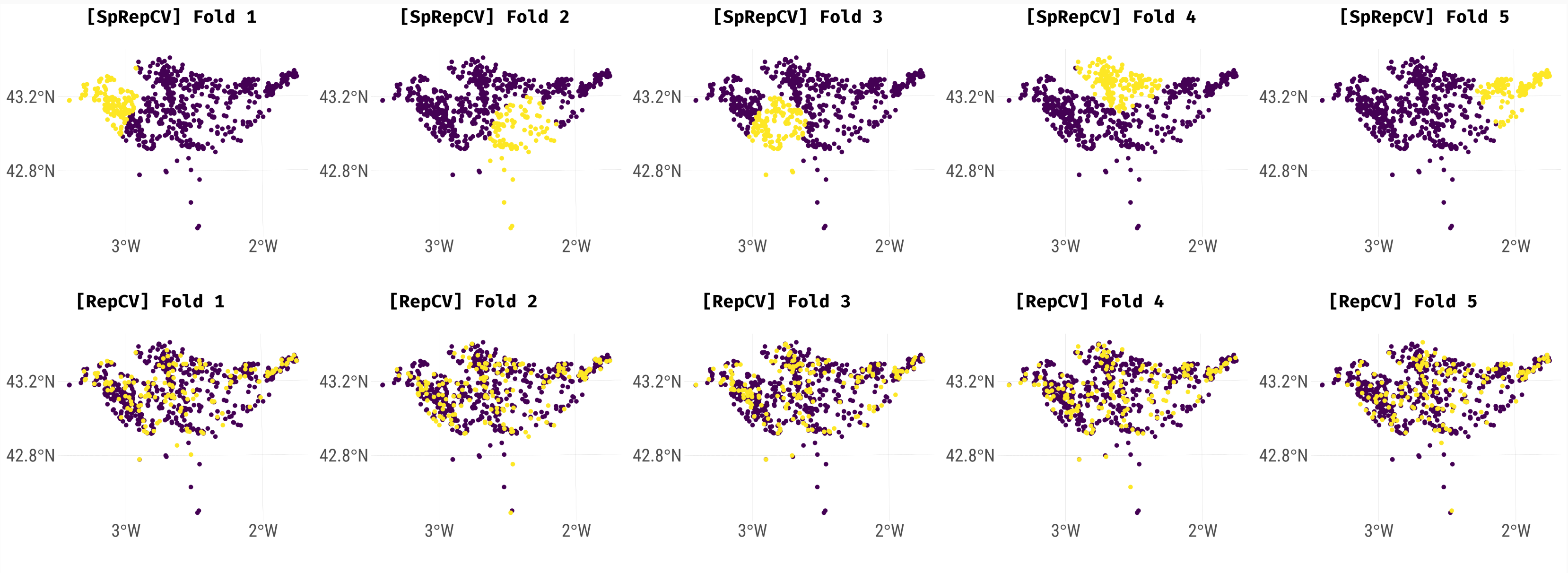

Fig. 4: Comparison of spatial and non-spatial partitioning of the data set.

Hyperparameter tuning

Random search has desirable properties in high dimensional and no disadvantages in low dimensional situations compared to **grid search** (Bergstra & Bengio, 2012).

Algorithm (package)	Hyperparameter	Type	Value	Start	End
BRT (gbm)	`n.tree`	integer	-	100	10000
	`shrinkage`	numeric	-	0	1.5
	`interaction.depth`	integer	-	1	40
RF (ranger)	`mtry`	integer	-	1	11
	`num.trees`	integer	-	10	10000
SVM (kernlab)	`C`	numeric	-	2^{-12}	2^{15}
	σ	numeric	-	2^{-15}	2^{6}
WKNN (kknn)	`k`	integer	-	10	400
	`distance`	integer	-	1	100
	`kernel`	nominal	*		

* triangular, Epanechnikov, biweight, triweight, cos, inv, Gaussian, optimal

Table 1: Hyperparameter limits and types of each model. Notations of hyperparameters from the respective R packages were used.

Results

Results

Hyperparameter tuning

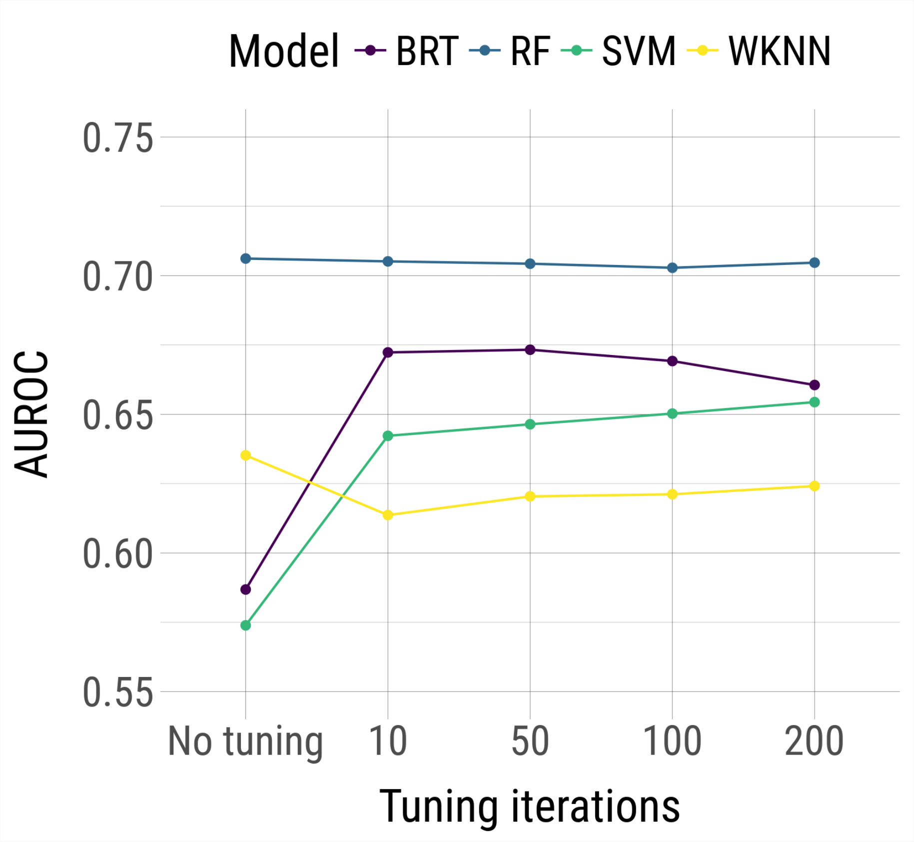

Fig 4: Hyperparameter tuning results of the spatial/spatial CV setting for BRT, WKNN, RF and SVM: Number of tuning iterations (1 iteration = 1 random hyperparameter setting) vs. predictive performance (AUROC).

Results (Predictive Performance)

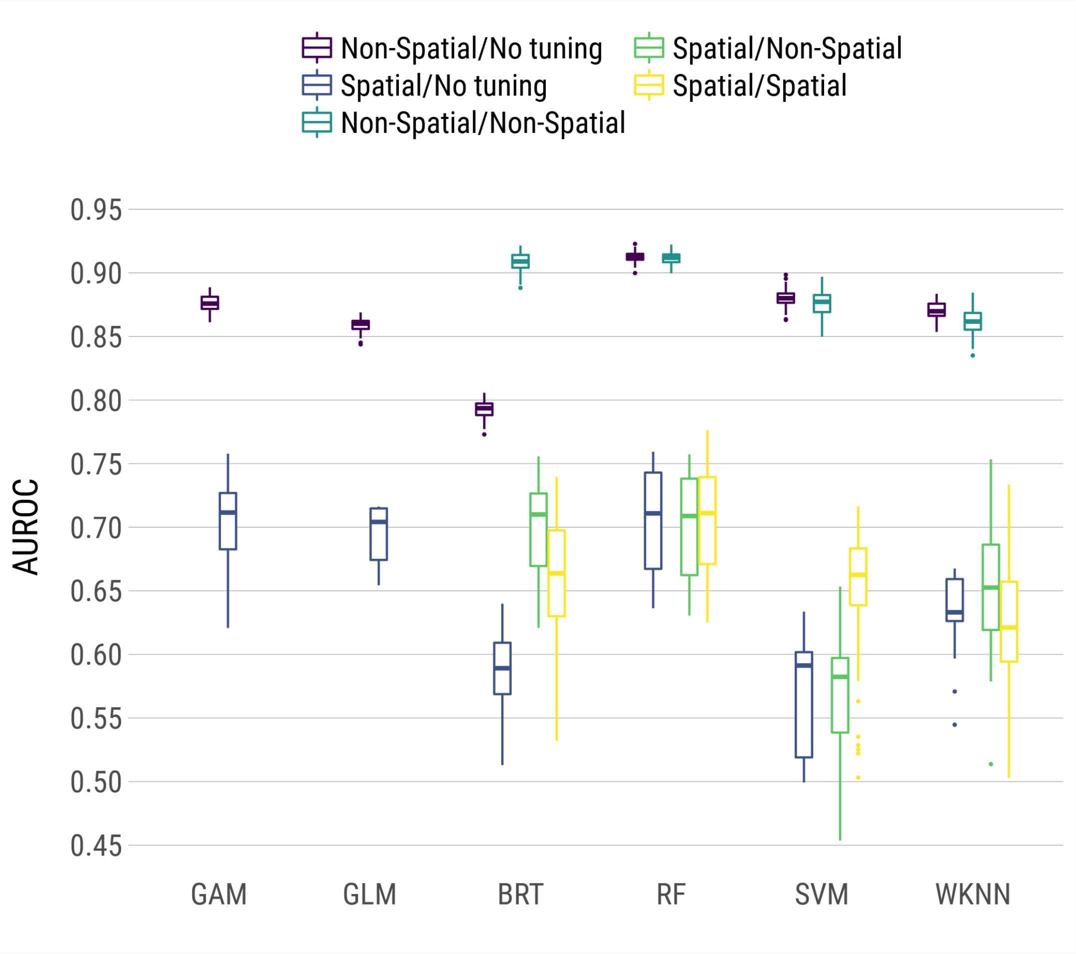

Fig 5: (Nested) CV estimates of model performance at the repetition level using 200 random search iterations. CV setting refers to perfomance estimation/hyperparameter tuning of the respective (nested) CV, e.g. ”Spatial/Non-Spatial” means that spatial partitioning was used for performance estimation and non-spatial partitioning for hyperparameter tuning.

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Predictive performance

- `RF` and `GAM` showed the best predictive performance

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- High bias in performance when using non-spatial CV

Discussion (Performance)

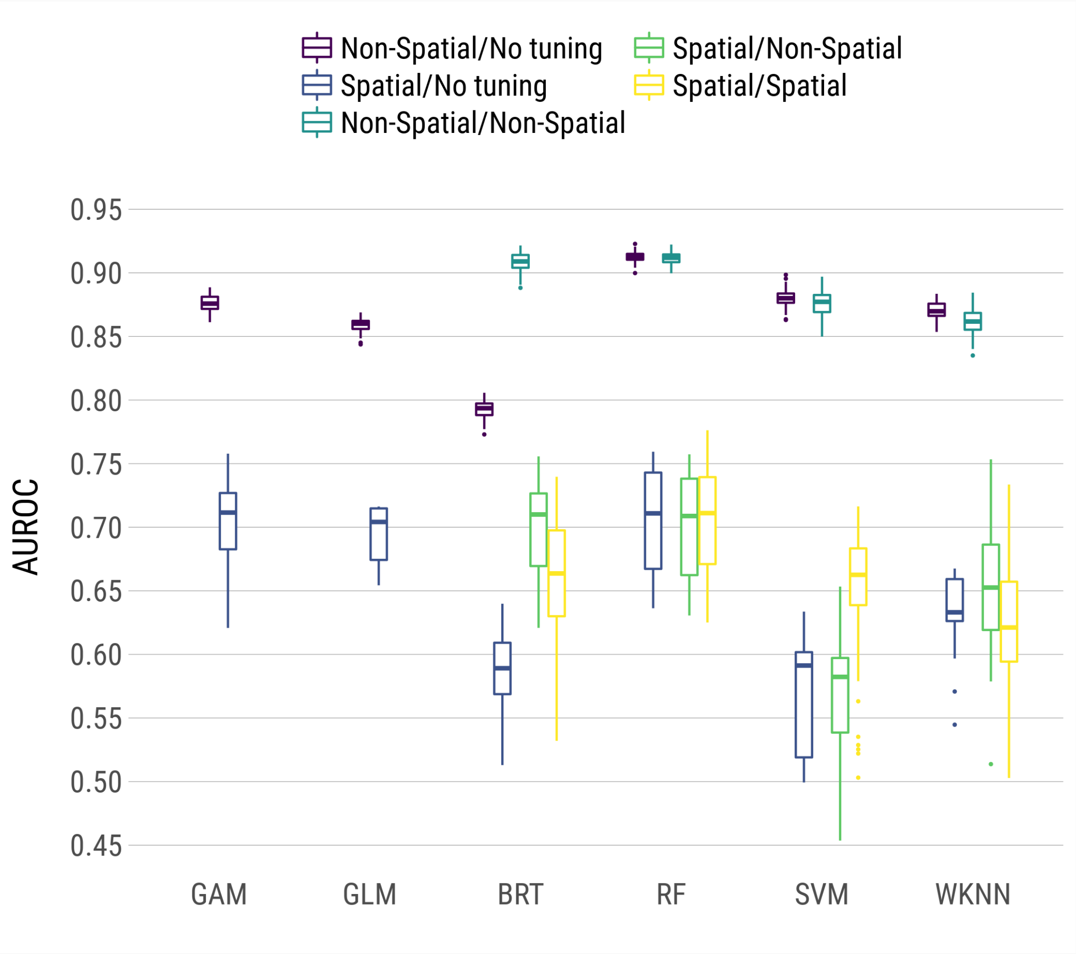

Fig 6: (Nested) CV estimates of model performance at the repetition level using 200 random search iterations. CV setting refers to perfomance estimation/hyperparameter tuning of the respective (nested) CV, e.g. "Spatial/Non-Spatial" means that spatial partitioning was used for performance estimation and non-spatial partitioning for hyperparameter tuning.

Predictive Performance

- `RF` and `GAM` showed the best predictive performance
- High bias in performance when using non-spatial CV
- Parametric models (`GLM`, `GAM`) show equally good performance estimates as the best ML algorithm (`RF`)

Discussion

Iturritxa et al. (2014)

GLM: 0.65 AUROC (without predictor `hail`)

GLM: 0.96 AUROC (with predictor `hail`)

This work

GLM: 0.66 AUROC (without predictor `hail_prob`) + slope, pH, lithology, soil

GLM: 0.694 (with predictor `hail_prob`) + slope, pH, lithology, soil

Discussion

Hyperparameter tuning

- Saturates at 50 repetitions and has a small effect for `SVM` and `BRT` (arbitrary defaults).

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- Almost no effect on predictive performance for WKNN and RF (reasonable defaults).
- Default hyperparameters of `RF` (and all other learners) are not suitable for spatial data

Discussion (Tuning)

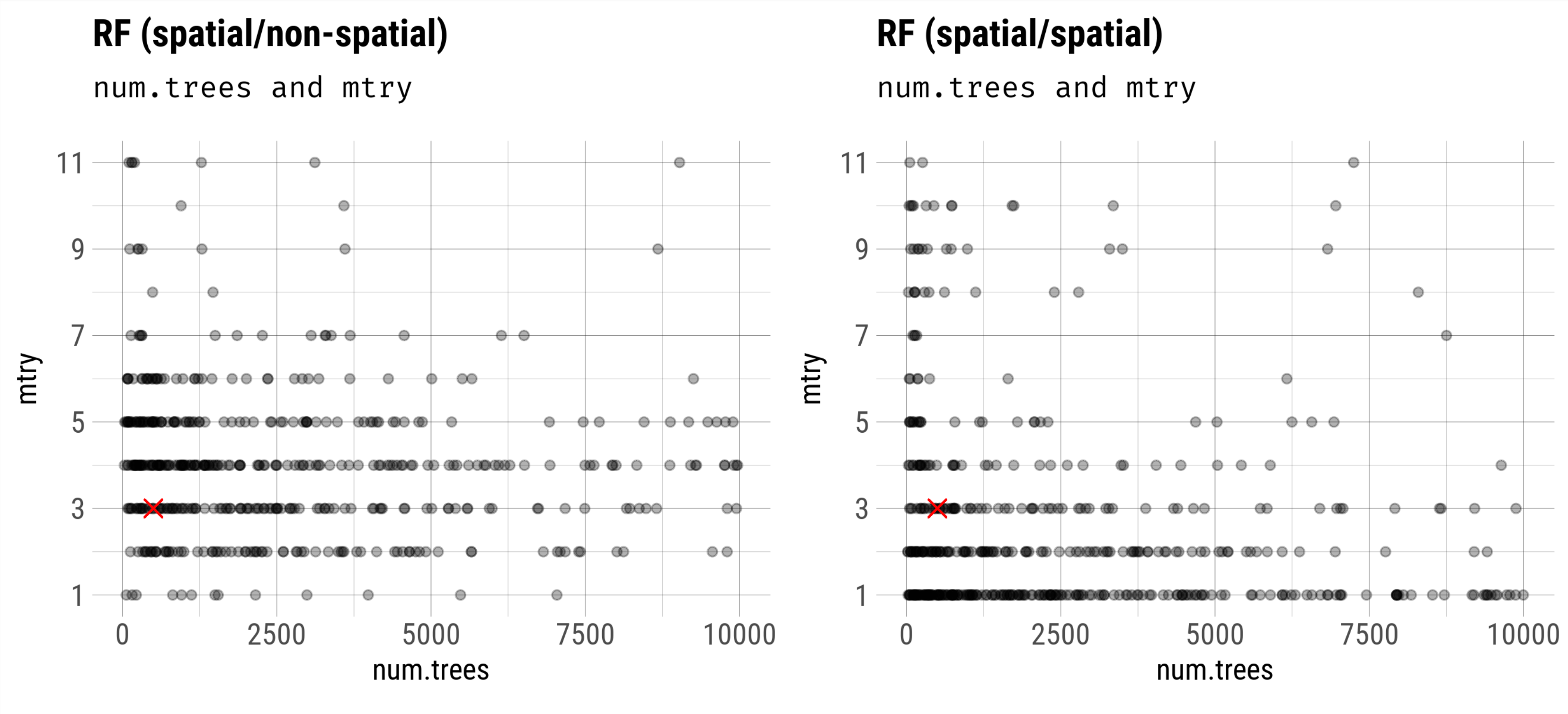


Fig 7: Best hyperparameter settings by fold (500 total) each estimated from 200 random search tuning iterations per fold using five-fold cross-validation. Split by spatial and non-spatial partitioning setup. Red crosses indicate default hyperparameter values. Black dots represent the winning hyperparameter setting out of each random search tuning of the respective fold.

Discussion

Hyperparameter tuning

- Saturates at ~ 50 repetitions and has a small effect for `SVM` and `BRT` (arbitrary defaults).
- Almost no effect for `WKNN` and `RF` (reasonable defaults).
- Default hyperparameters of `RF` (and all other learners) are not suitable for spatial data
    - They **possibly** lead to biased performance estimates as they cause fitted models to make use of the remaining spatial autocorrelation in the data.
    - Meaningful default values (`RF`, `WKNN`) have been estimated on non-spatial data sets.

❗ Always perform a spatial hyperparameter tuning for spatial data sets, even if it does not improve accuracy ❗

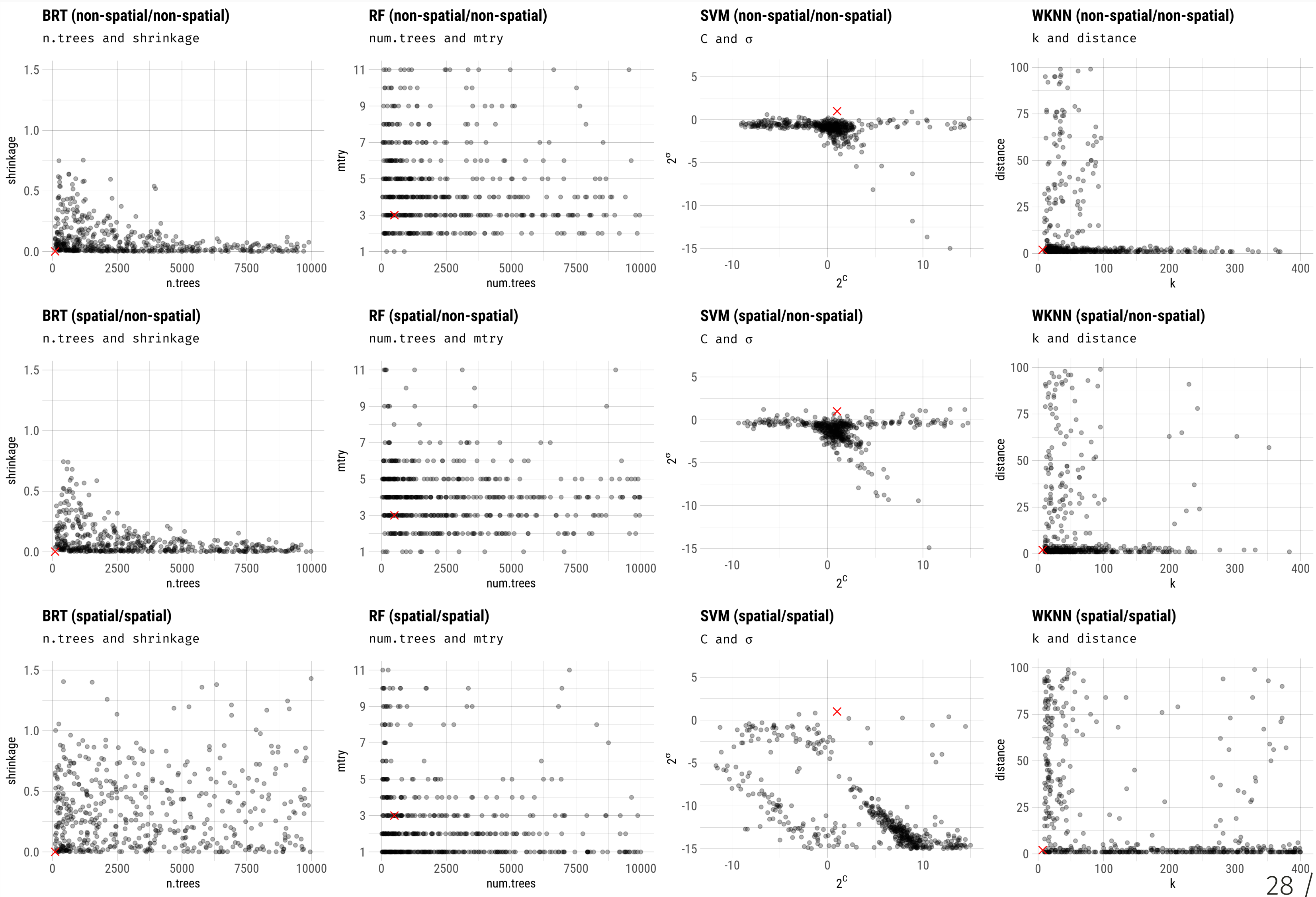
References

Bergstra, J., & Bengio, Y. (2012). Random search for hyperparameter optimization. J. Mach. Learn. Res., 13, 281–305. URL: http://dl.acm.org/citation.cfm?id=2188385.2188395.

Iturritxa, E., Mesanza, N., & Brenning, A. (2014). Spatial analysis of the risk of major forest diseases in Monterey pine plantations. Plant Pathology, 64, 880–889. doi:10.1111/ppa.12328.

Backup ➕

Backup



BRT (non-spatial/non-spatial)
n.trees and shrinkage
shrinkage
n.trees
RF (non-spatial/non-spatial)
num.trees and mtry
mtry
num.trees
SVM (non-spatial/non-spatial)
C and σ
2^{σ}
2^{C}
WKNN (non-spatial/non-spatial)
k and distance
distance
k
BRT (spatial/non-spatial)
n.trees and shrinkage
shrinkage
n.trees
RF (spatial/non-spatial)
num.trees and mtry
mtry
num.trees
SVM (spatial/non-spatial)
C and σ
2^{σ}
2^{C}
WKNN (spatial/non-spatial)
k and distance
distance
k
BRT (spatial/spatial)
n.trees and shrinkage
shrinkage
n.trees
RF (spatial/spatial)
num.trees and mtry
mtry
num.trees
SVM (spatial/spatial)
C and σ
2^{σ}
2^{C}
WKNN (spatial/spatial)
k and distance
distance
k

Backup

Table 2: Mean AUROC (repetition level) for different 5-fold 100 times repeated cross-validation settings. Settings with tuning are based on 200 random search iterations. Highest values of each column are highlighted in bold.

Performance estimation	Non-Spatial		Spatial		
Hyperparameter tuning	Non-Spatial	Non	Non-Spatial	Spatial	Non
GLM	-	0.859	-	-	0.694
GAM	-	**0.876**	-	-	0.705
BRT	0.909	-	0.699	0.661	0.587
RF	**0.911**	-	**0.702**	**0.705**	**0.706**
SVM	0.876	-	0.566	0.654	0.574
WKNN	0.861	-	0.652	0.624	0.635