RETHINKING VALIDATION FOR SPATIAL MACHINE LEARNING

Jakub Nowosad (Adam Mickiewicz University, Poznań and University of Münster)
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Roles of spatial machine learning?

Explanatory: understanding the world

Predictive: forecasting the future or mapping the present

Both: understanding the world to map the present/future *(holy grail)*

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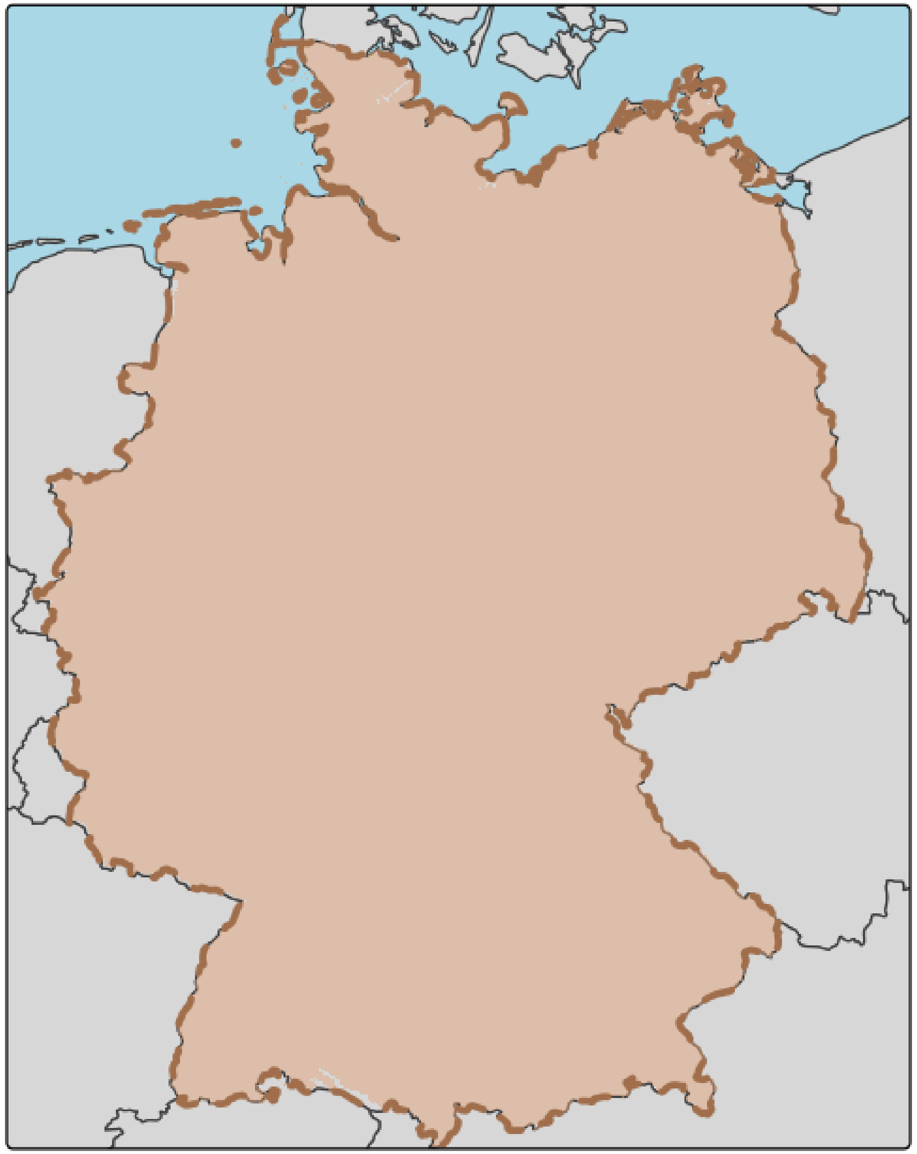
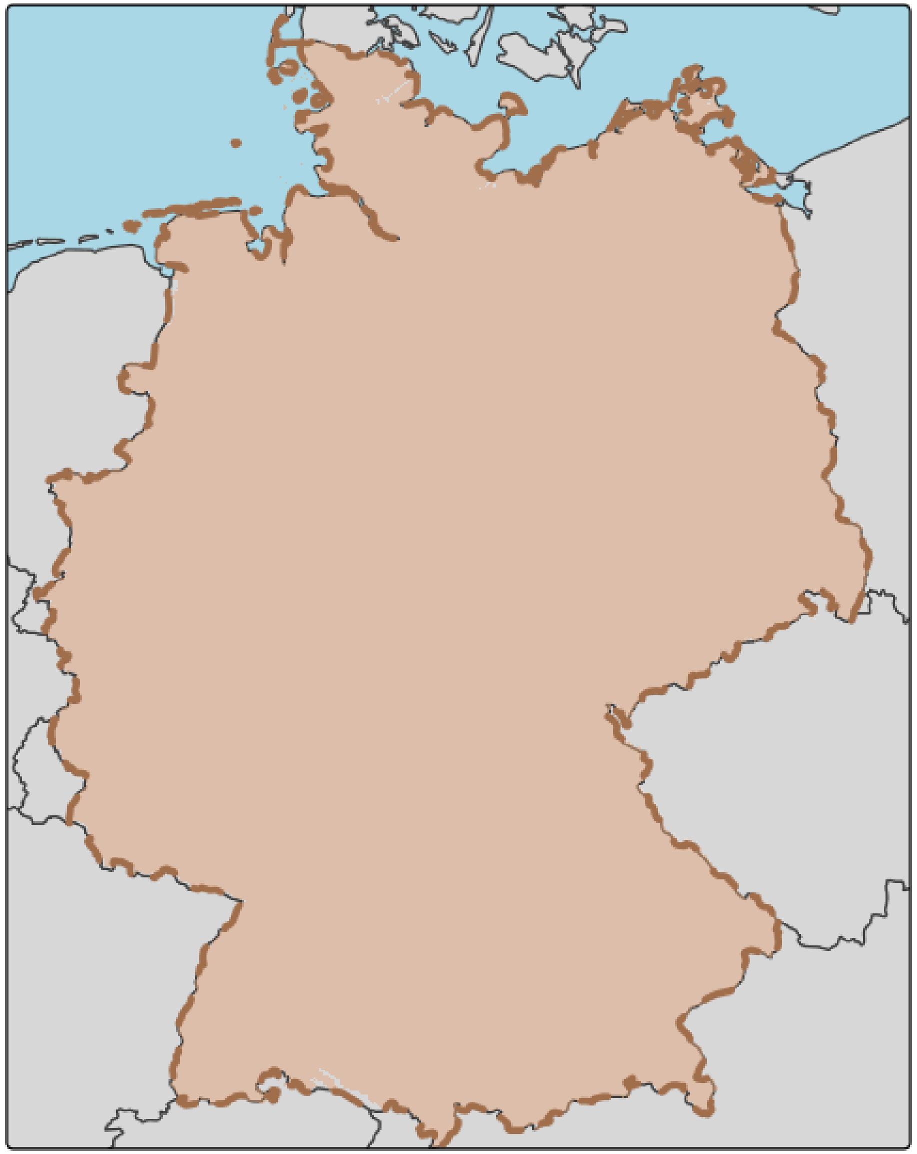
Predictive spatial machine learning



Prediction domain

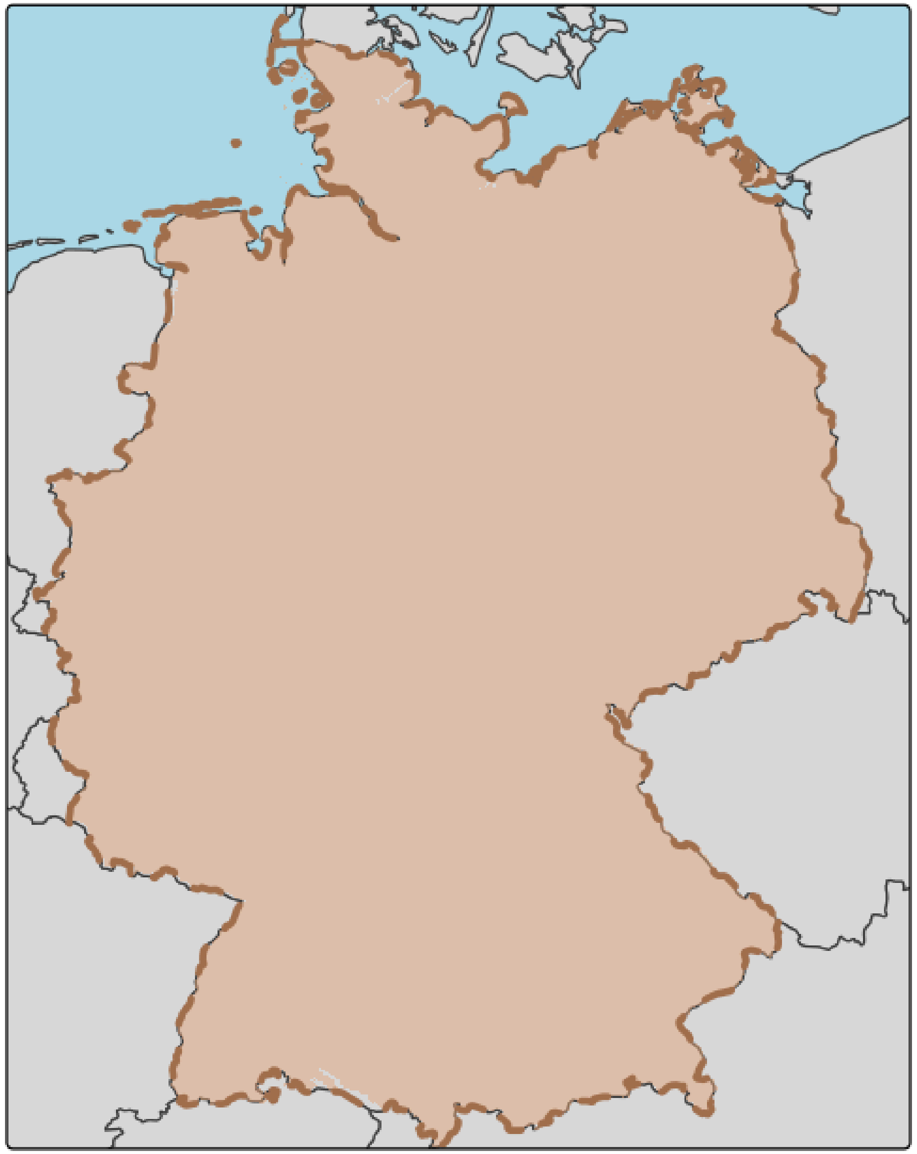
Predictive spatial machine learning



Prediction domain

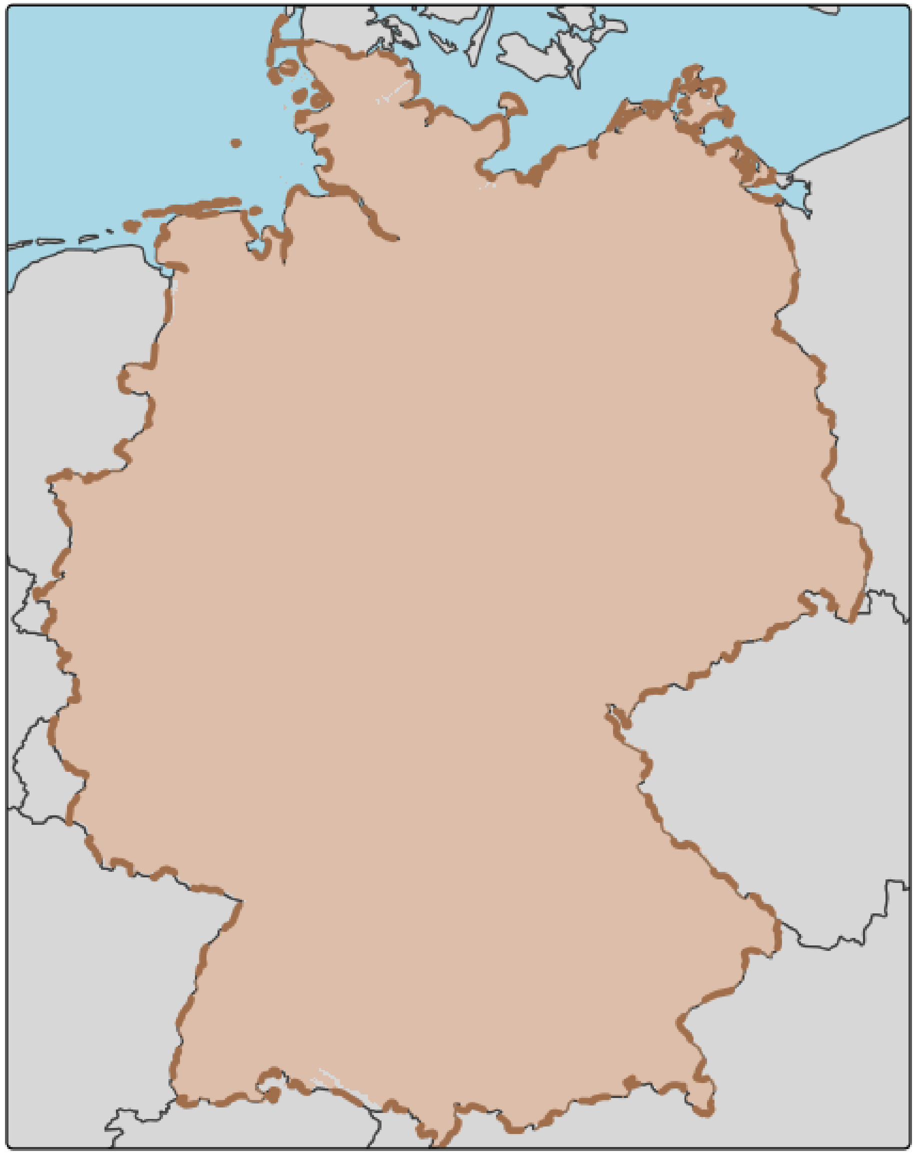
- We are interested in mapping across the spatial domain

Predictive spatial machine learning



Prediction domain

- We are interested in mapping across the spatial domain
- Thus, we should evaluate the map, not the model



Prediction domain

Predictive spatial machine learning

- We are interested in mapping across the spatial domain
- Thus, we should evaluate the map, not the model
- **But this raises a key question:** *What assumptions are we making about spatial evaluation?*

ASSUMPTION #1

Assumptions we make

We can predict everywhere

Assumptions we make

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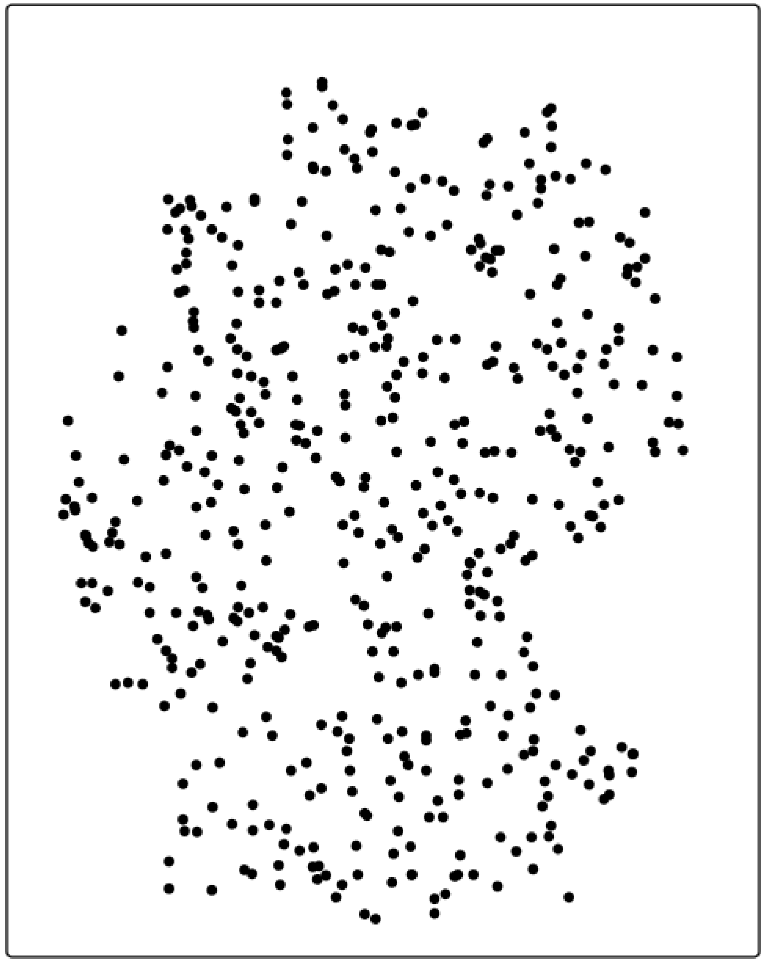
Reality:

We validate where we have data, but predict where we do not.

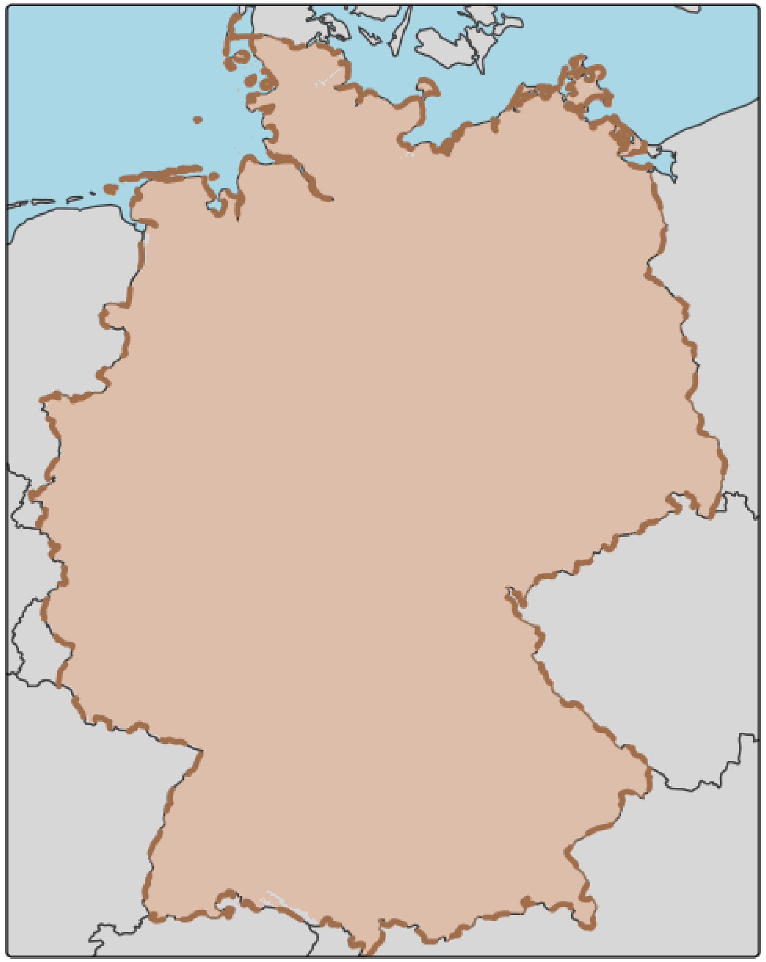
Similar application domain

We have this:



Sampling locations

We want to predict here:



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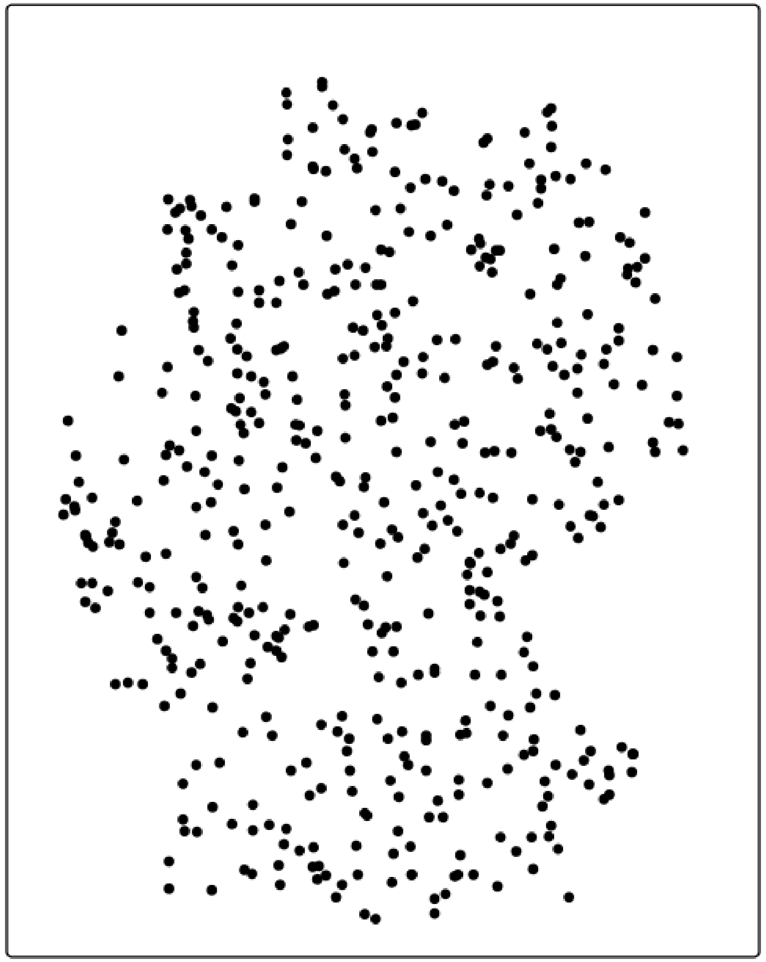

Sampling locations

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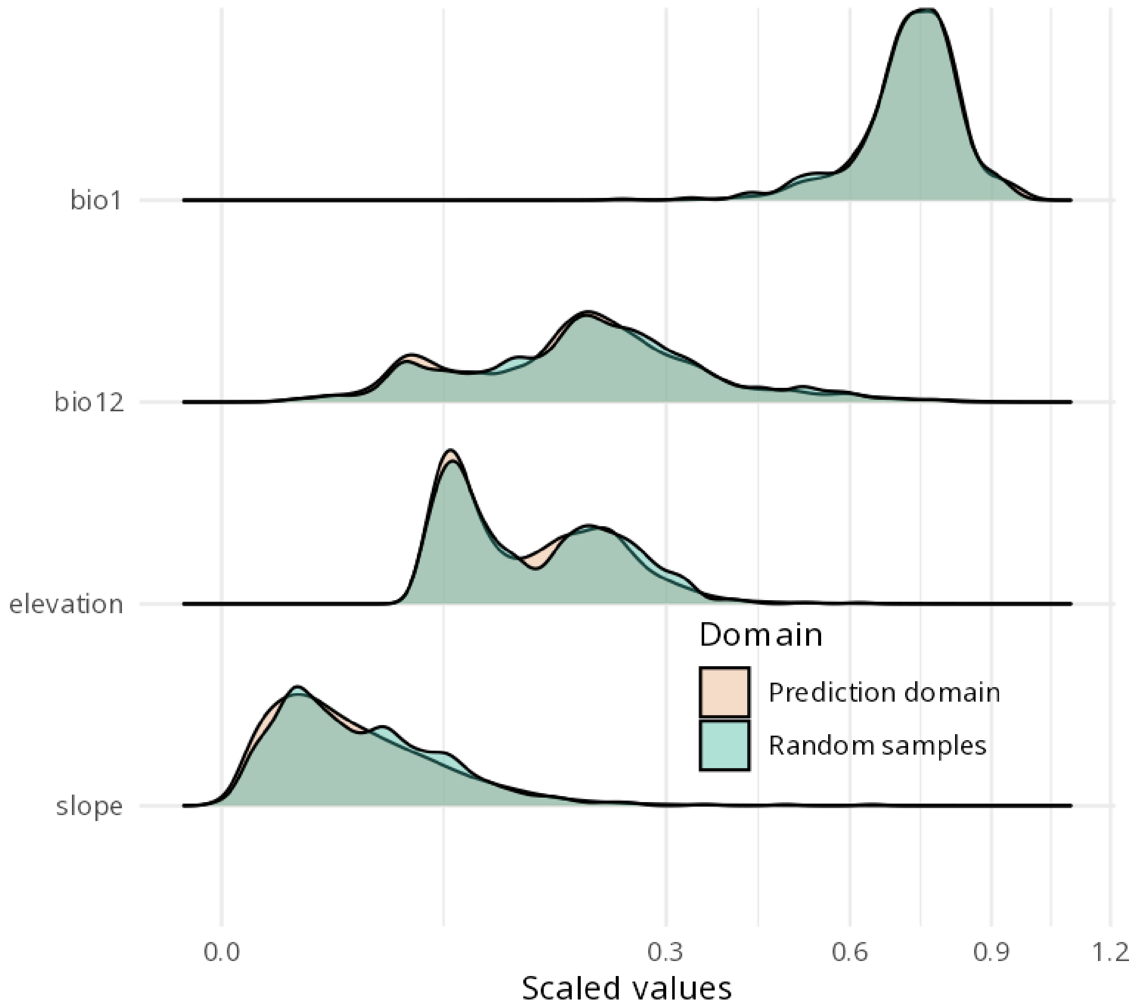

Different application domain

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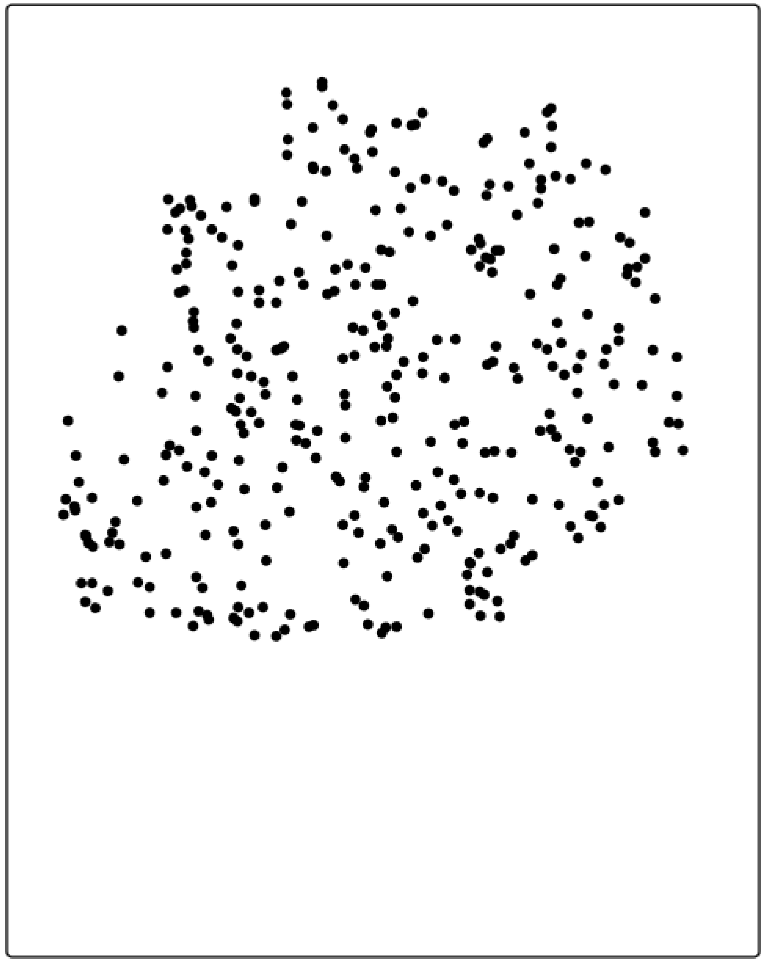

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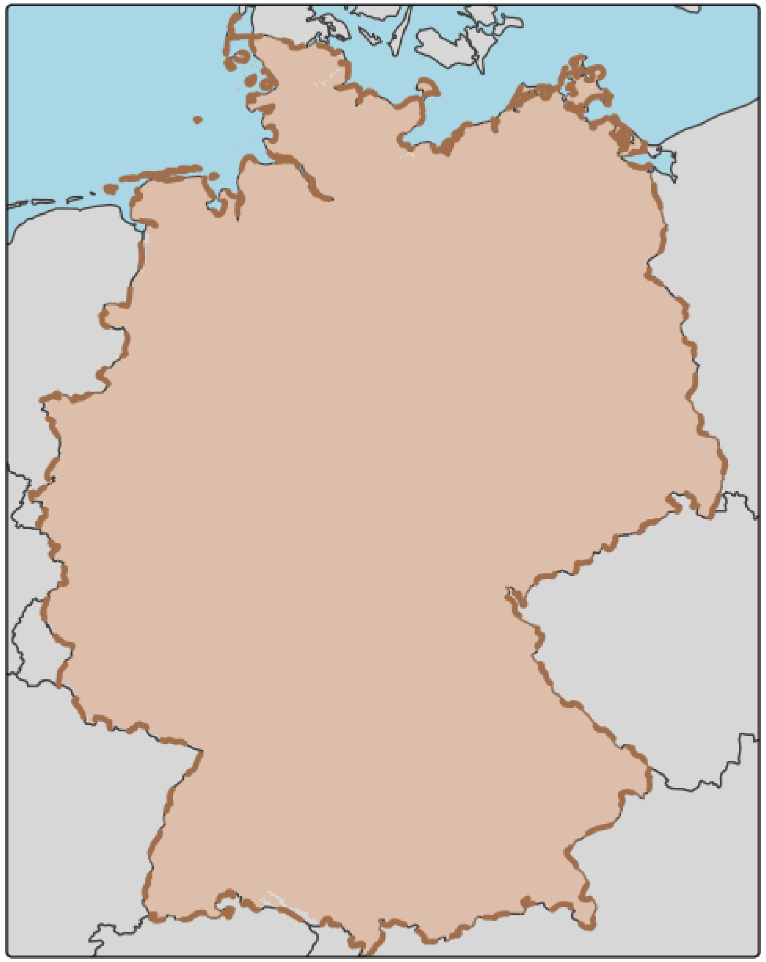

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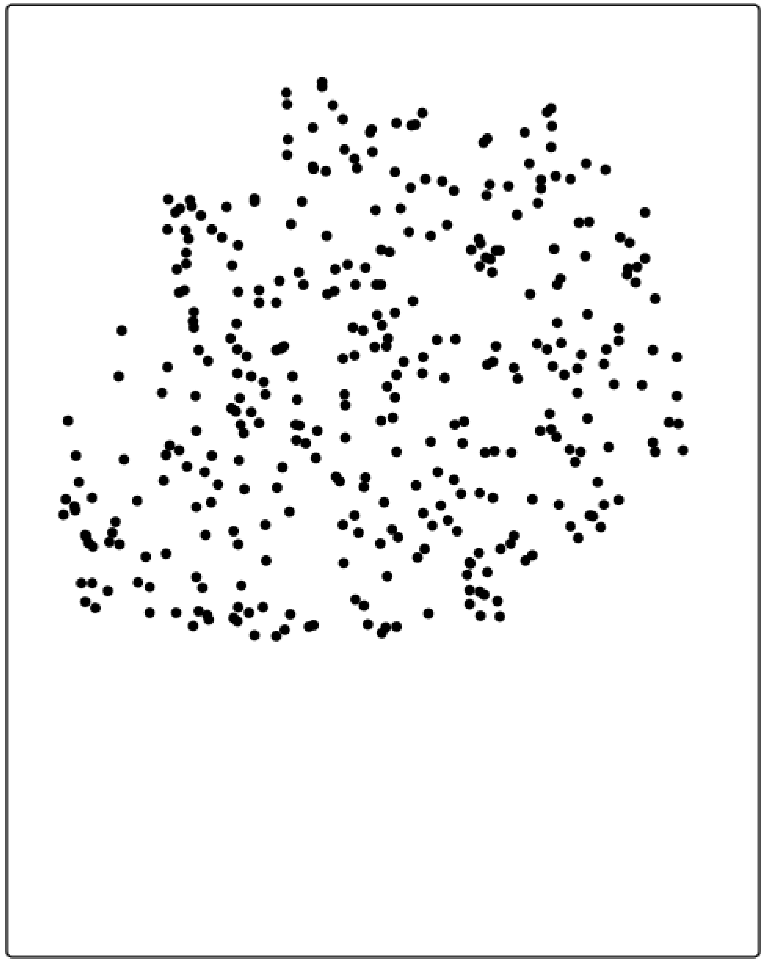

Sampling locations

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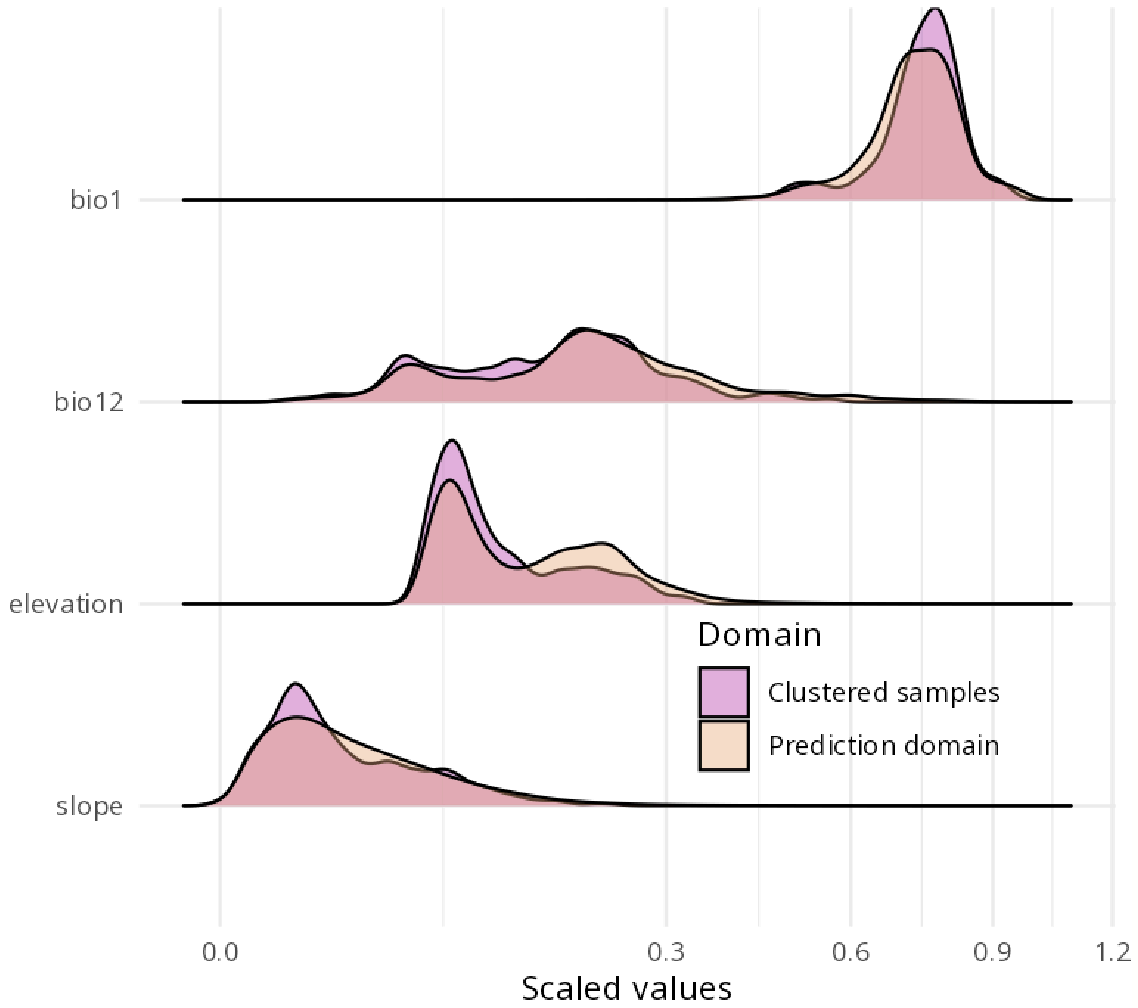
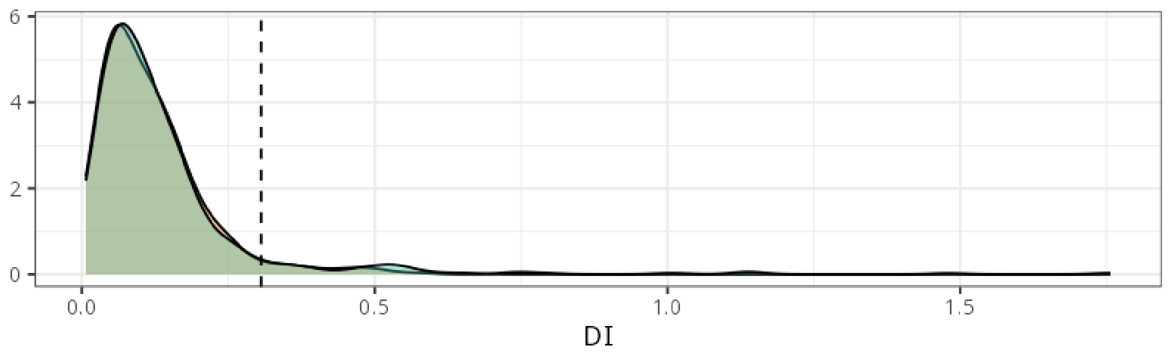
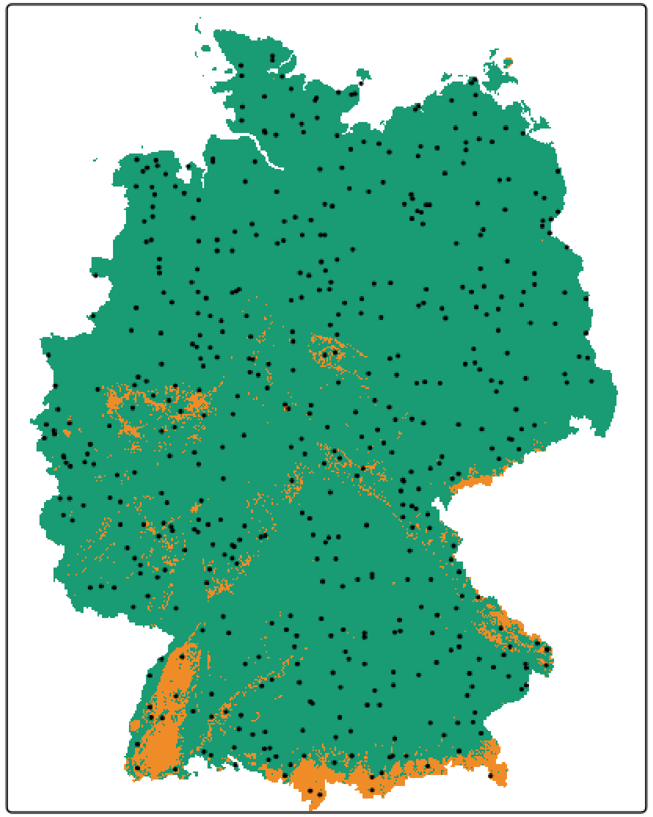
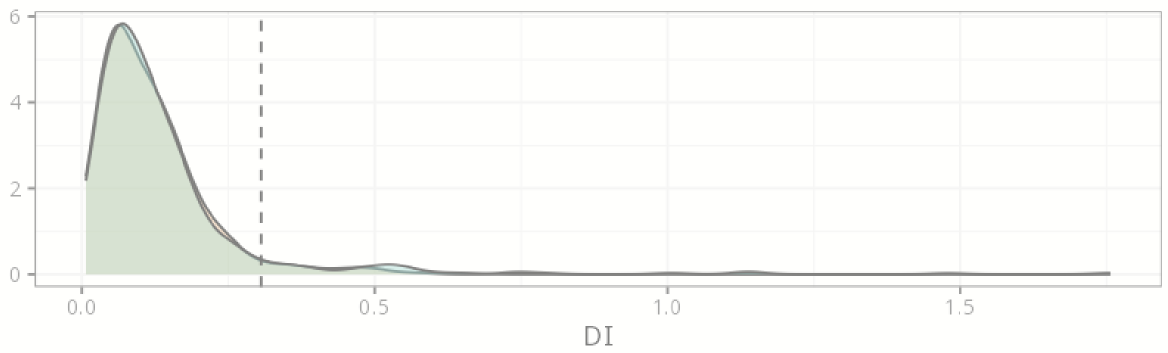




Random samples (93.9% inside AOA)





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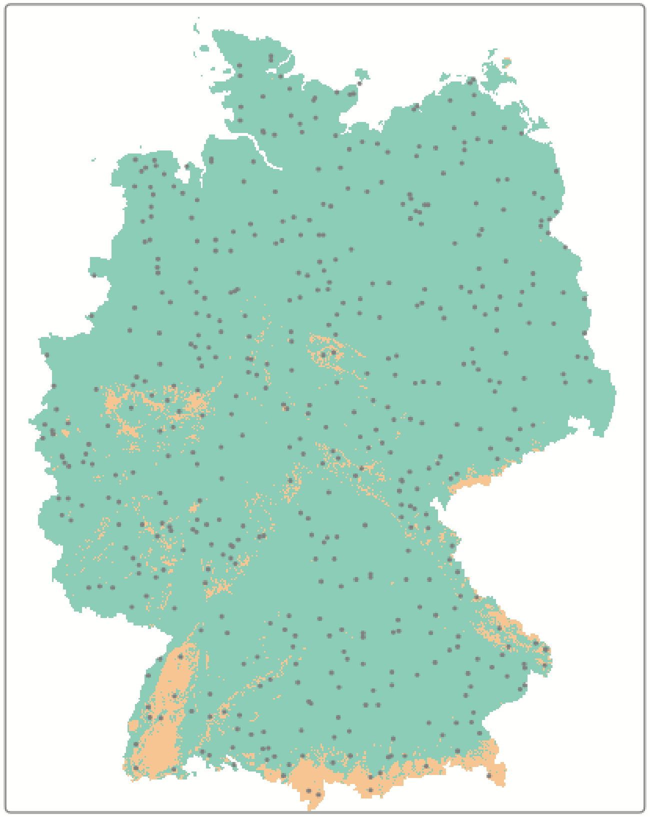

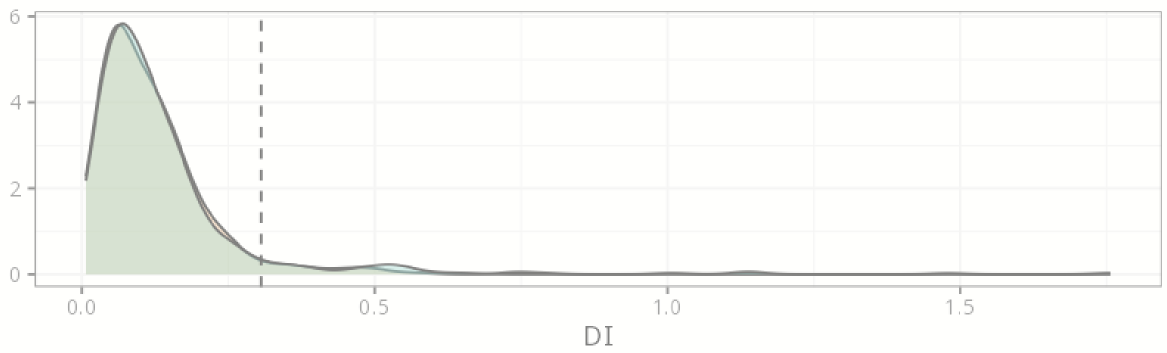

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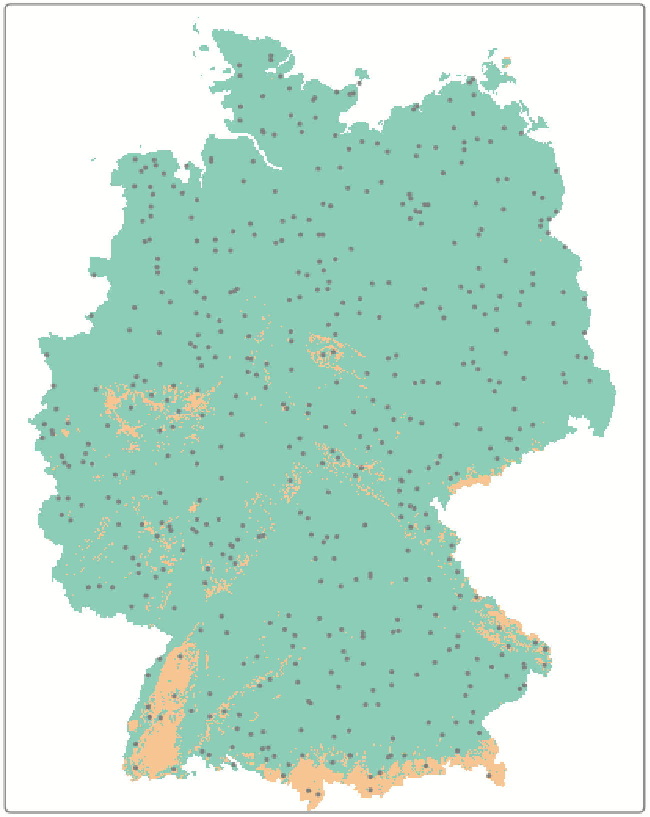
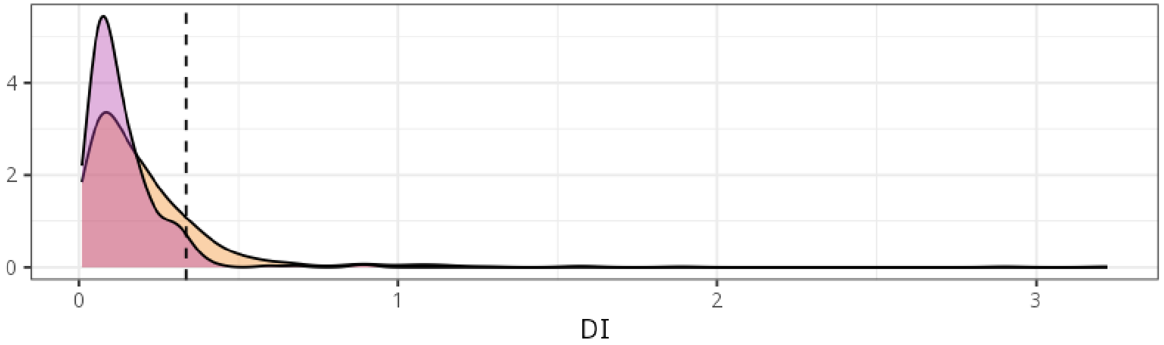
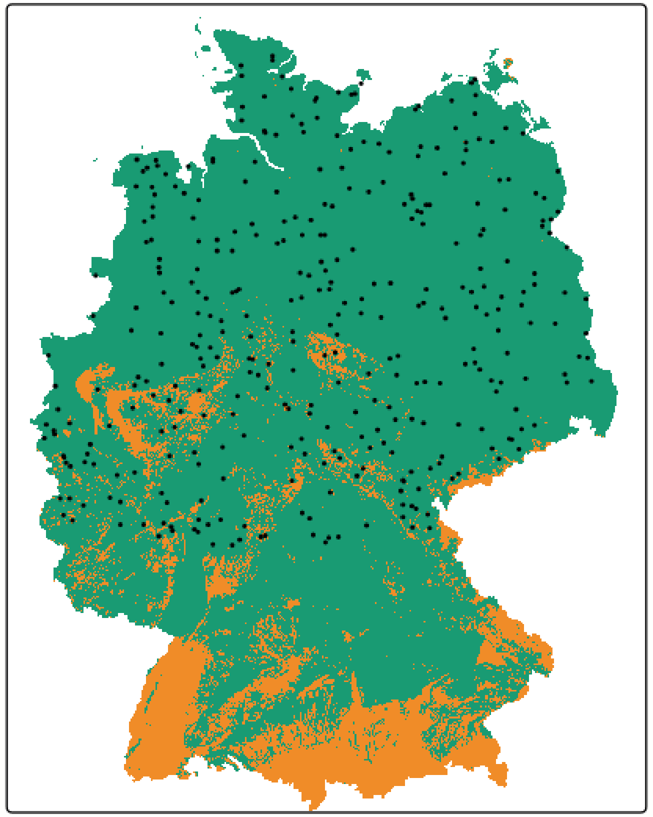




Partitioned samples (83.9% inside AOA)



Area of applicability

Identify areas where the environment is not well represented, making predictions less trustworthy (Area of Applicability – AoA, Meyer and Pebesma, 2021); also local point density (LPD, Schumacher et al., 2025)

See also: MESS, Elith et al., 2010, Jung et al., 2020, and Velazco et al., 2023 for other related approaches

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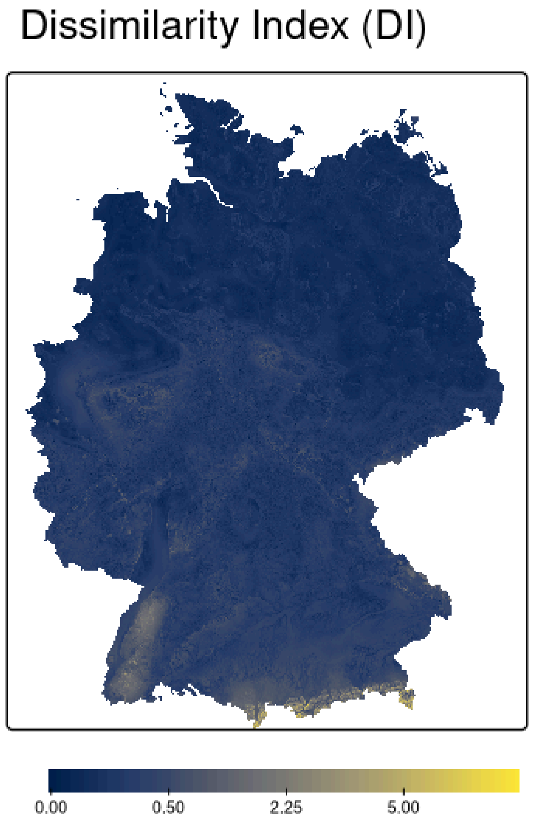

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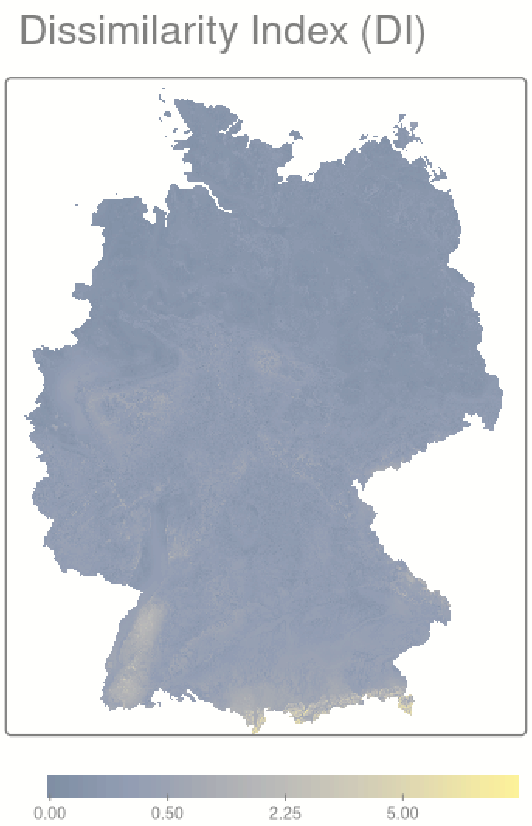

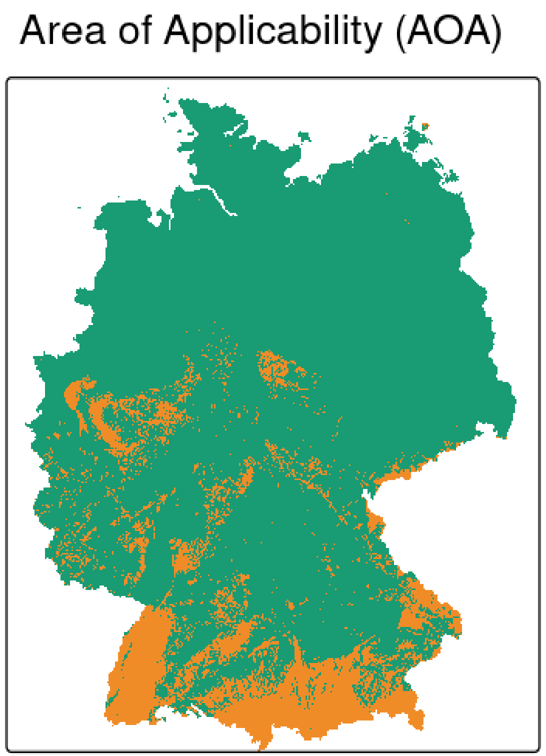

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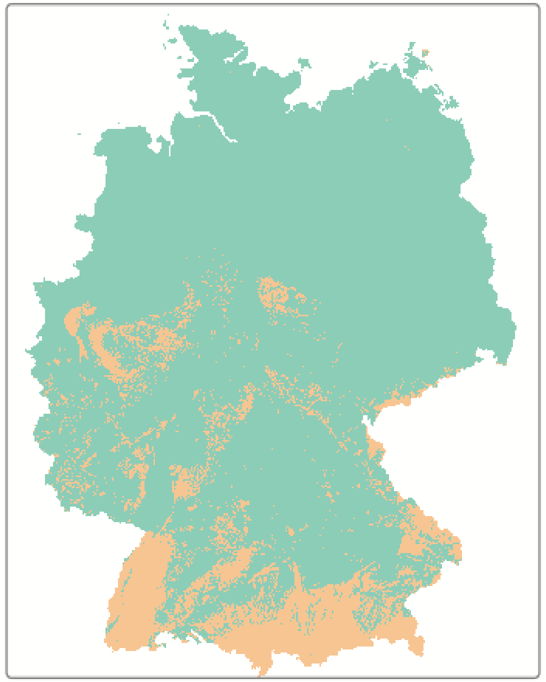
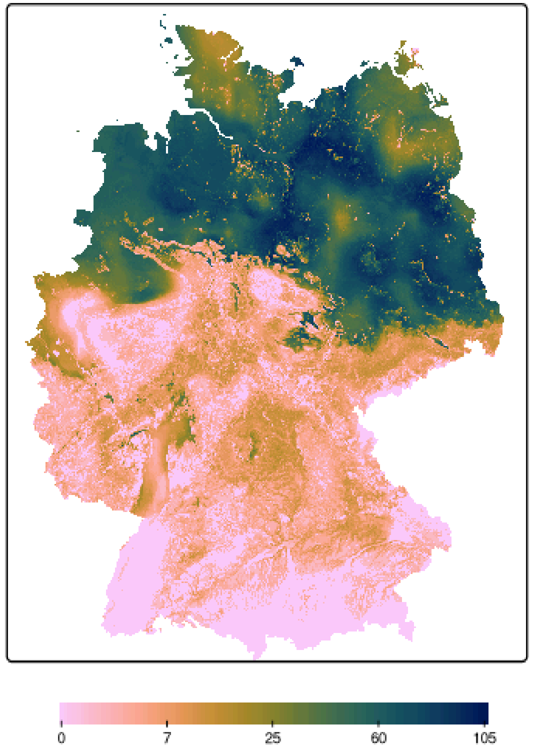
Dissimilarity Index (DI)

Area of Applicability (AOA)



Local Point Density (LPD)



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ASSUMPTION #2

Assumptions we make

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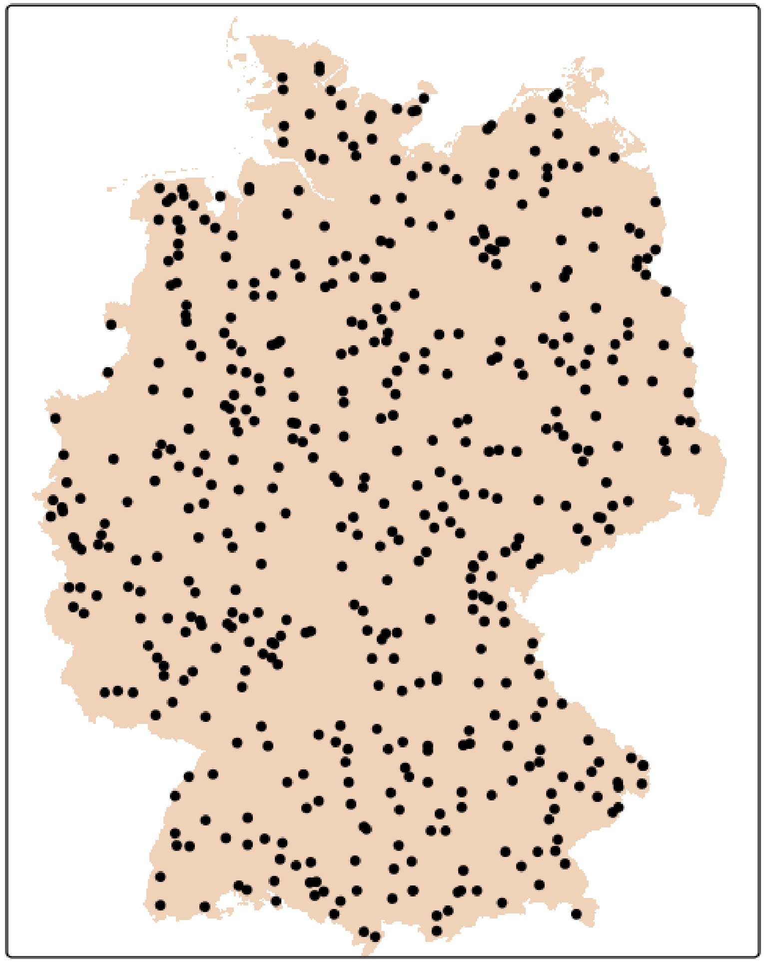
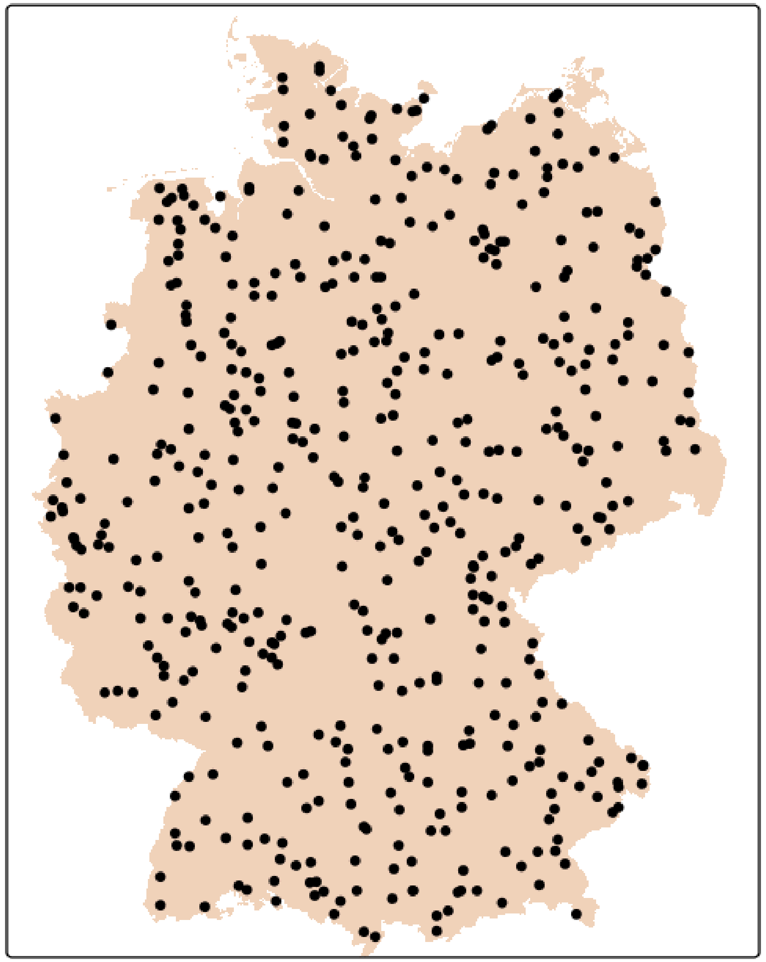
Prediction difficulty depends on prediction domain



Random sampling locations

Prediction difficulty depends on prediction domain



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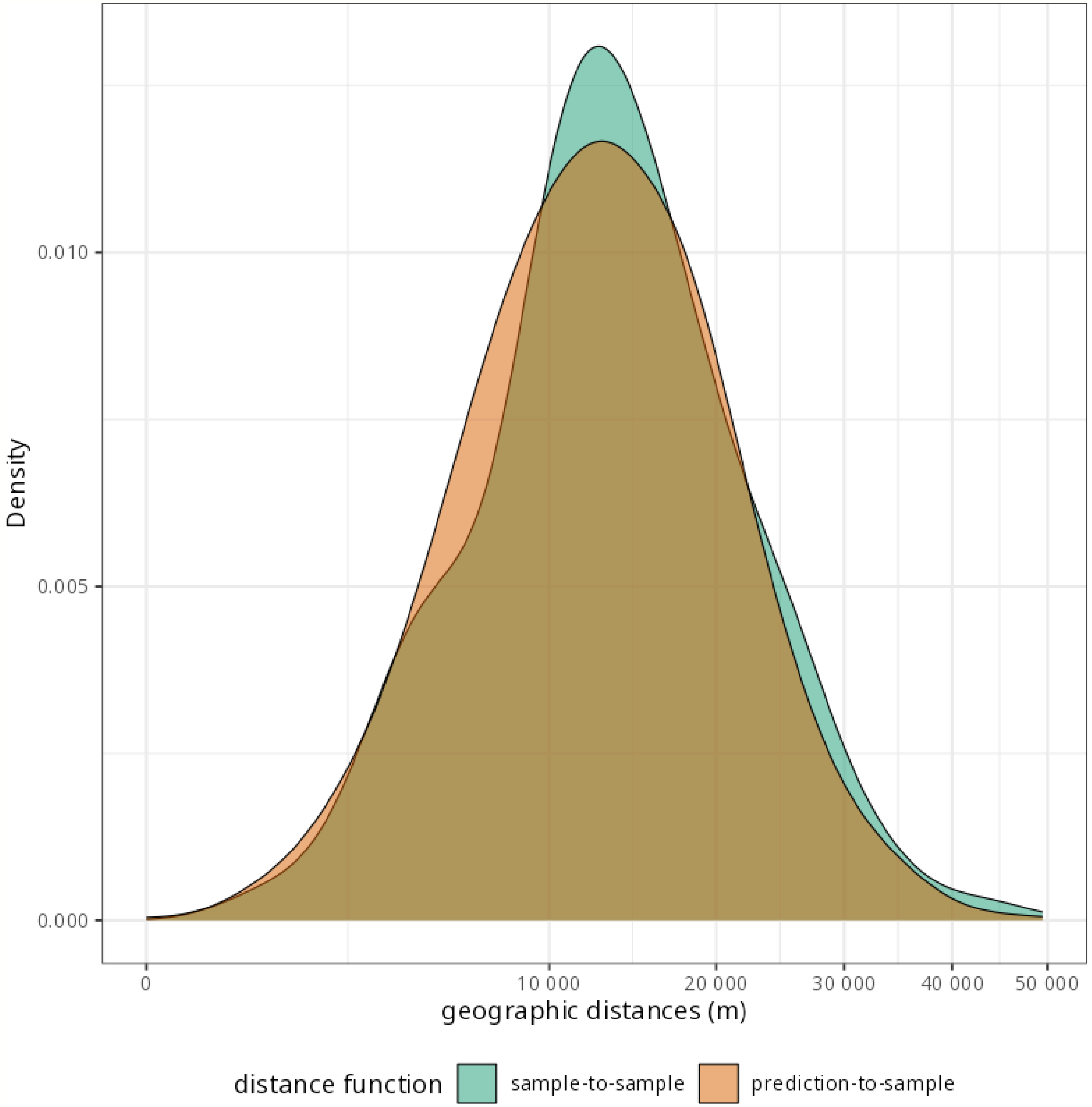

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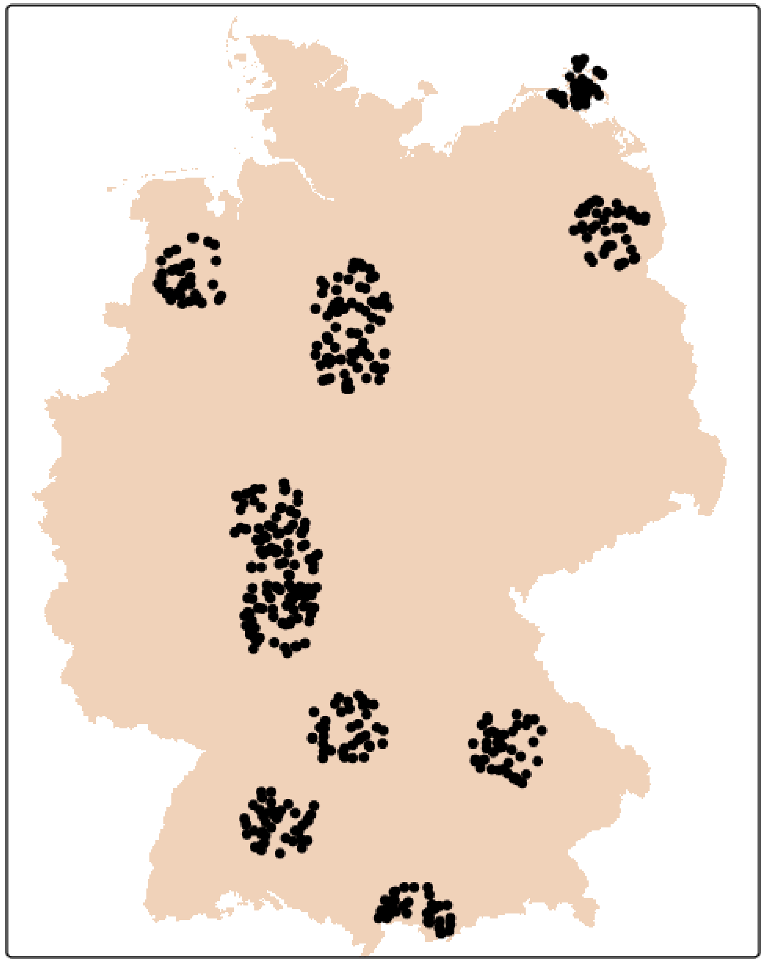

Clustered sampling locations

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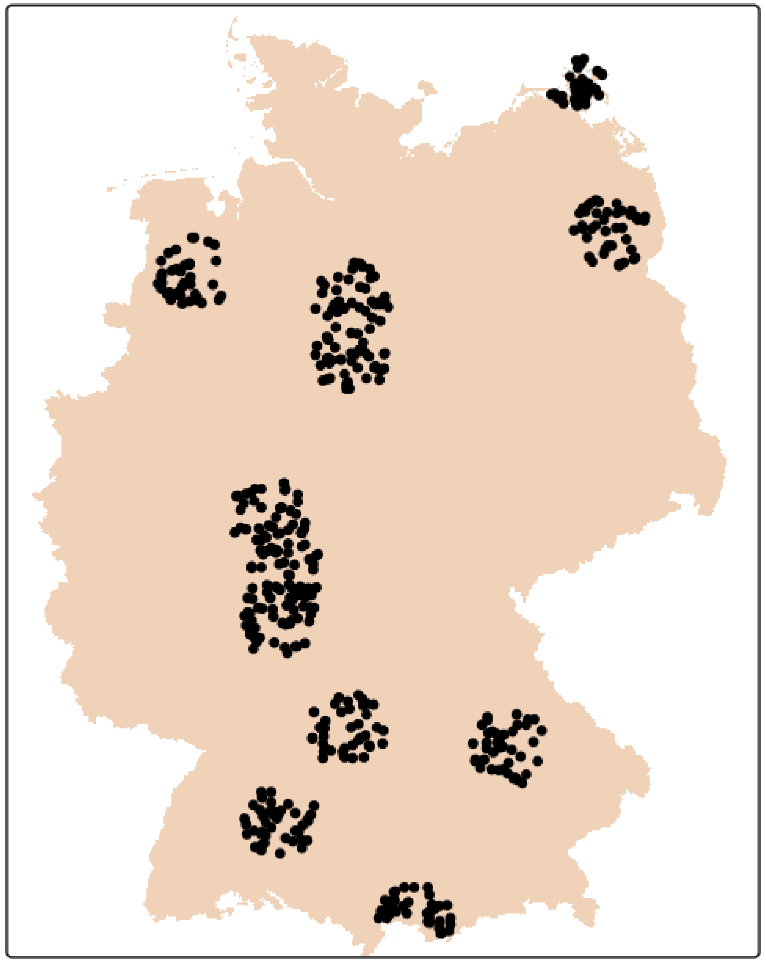

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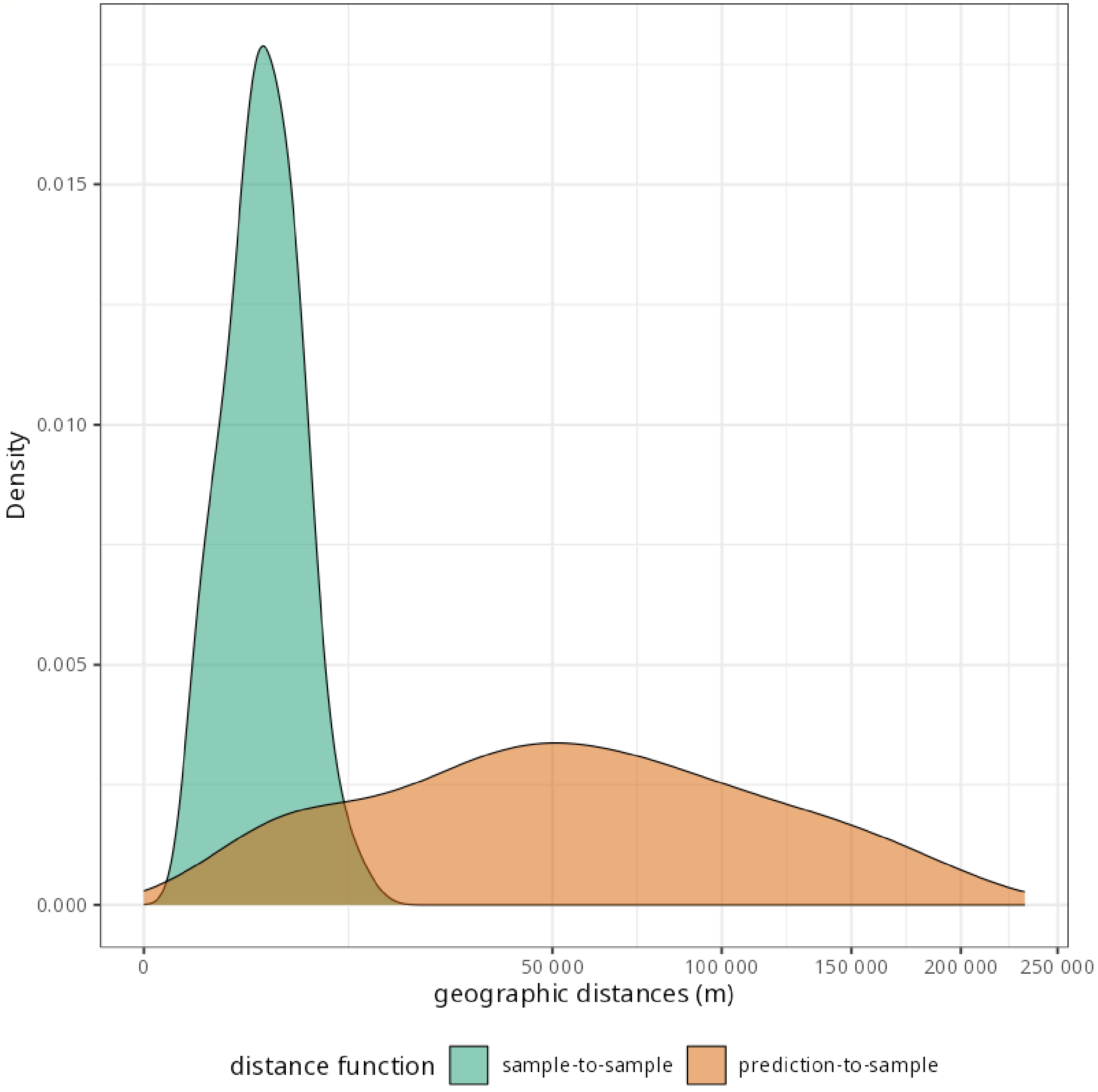
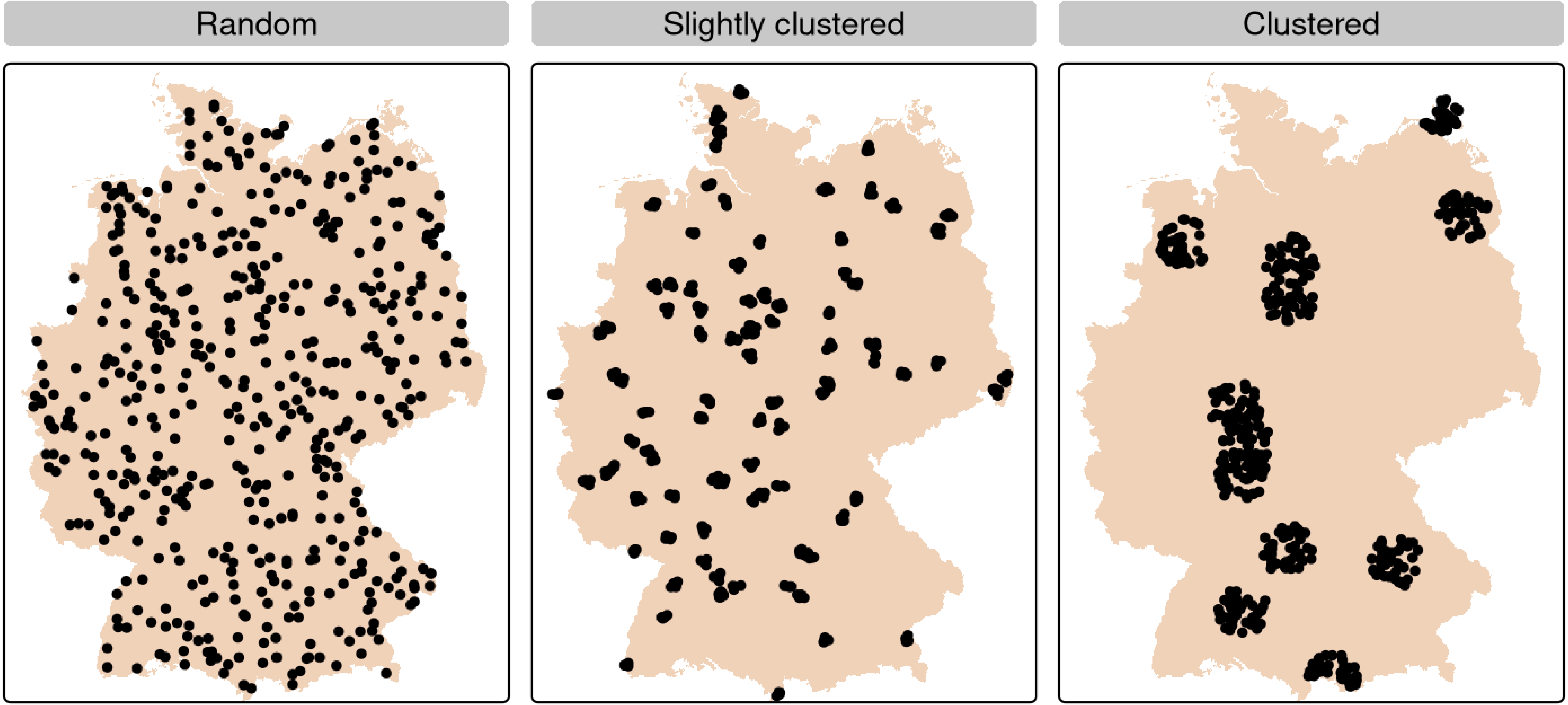
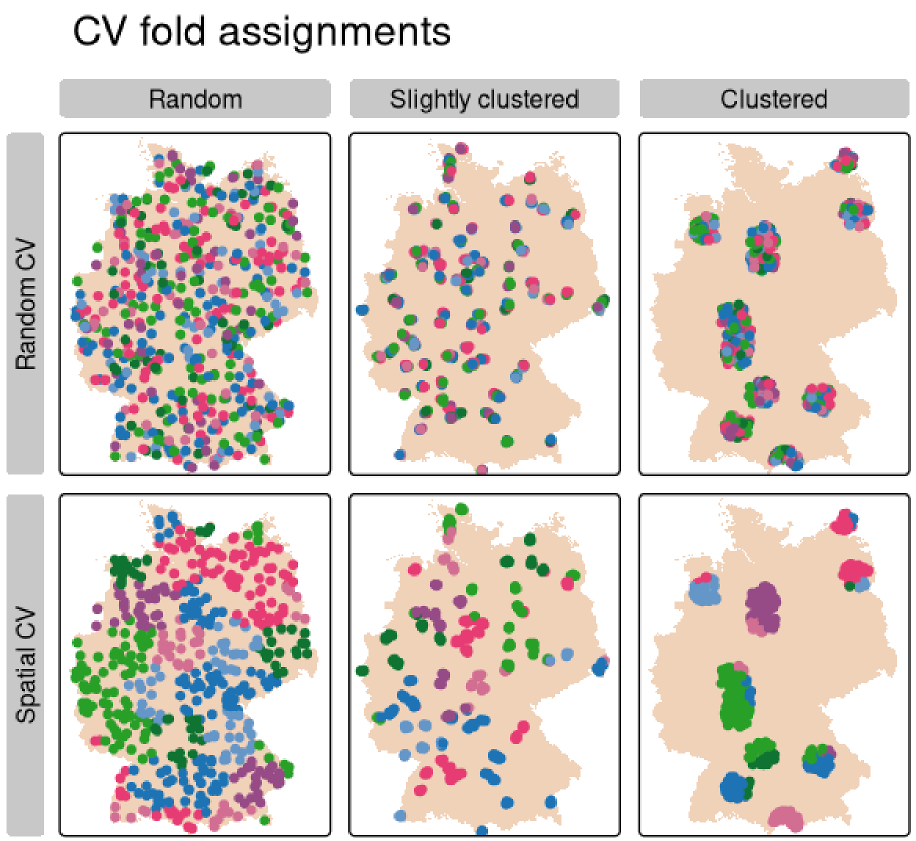


Extrapolation continuum



Specific evaluation strategy



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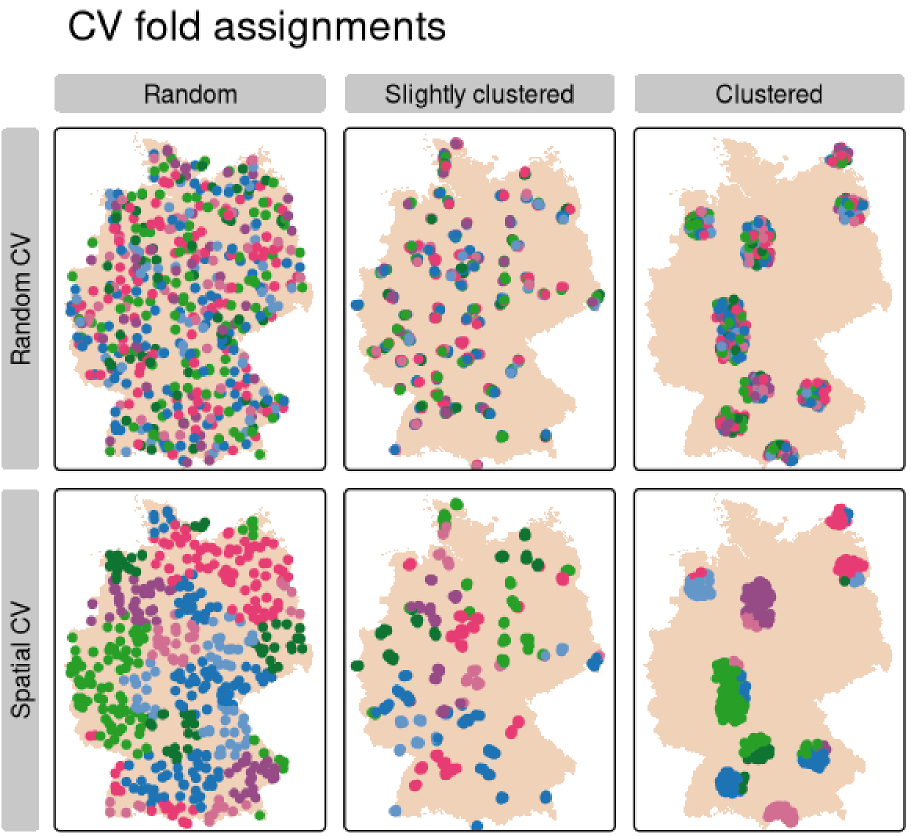
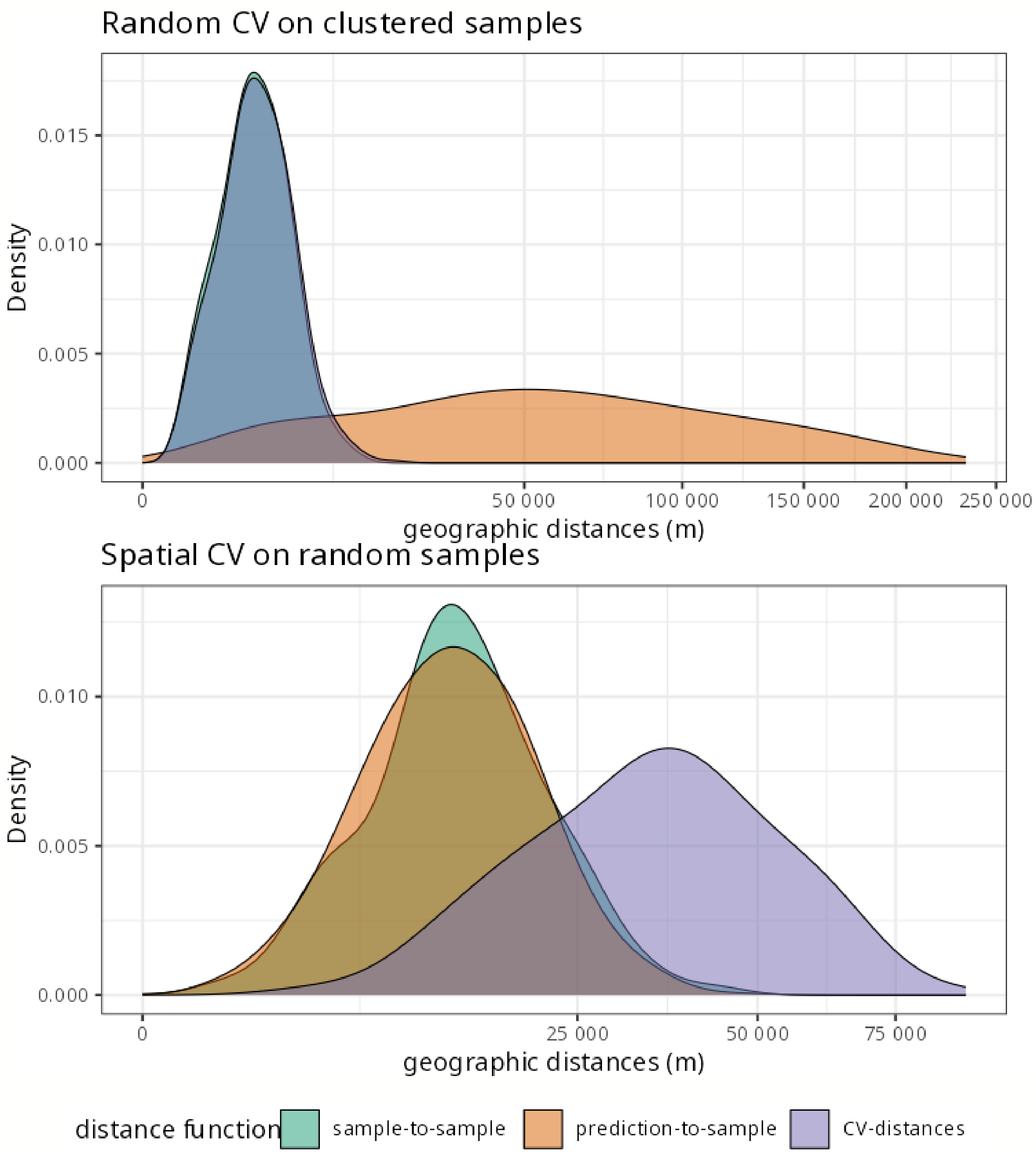
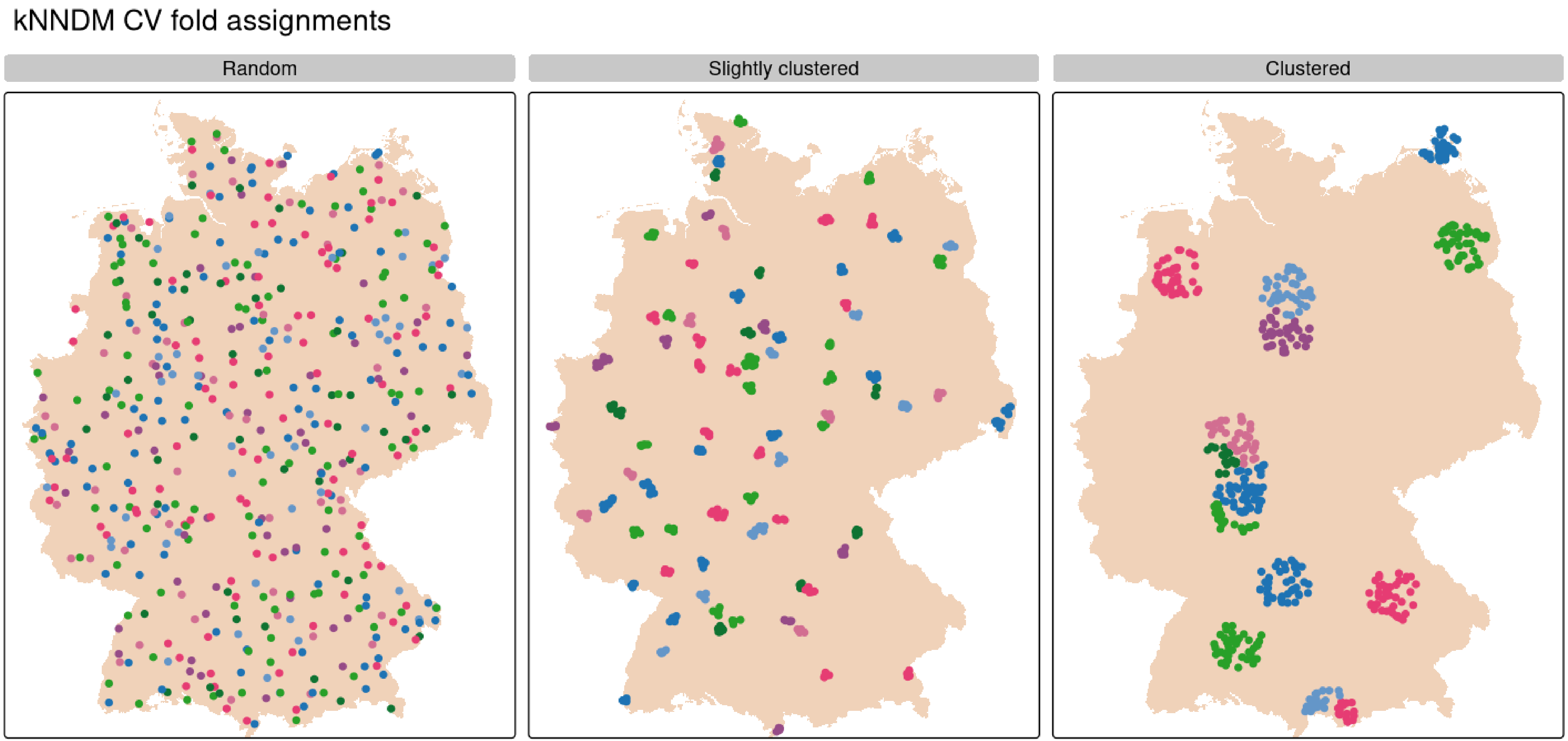
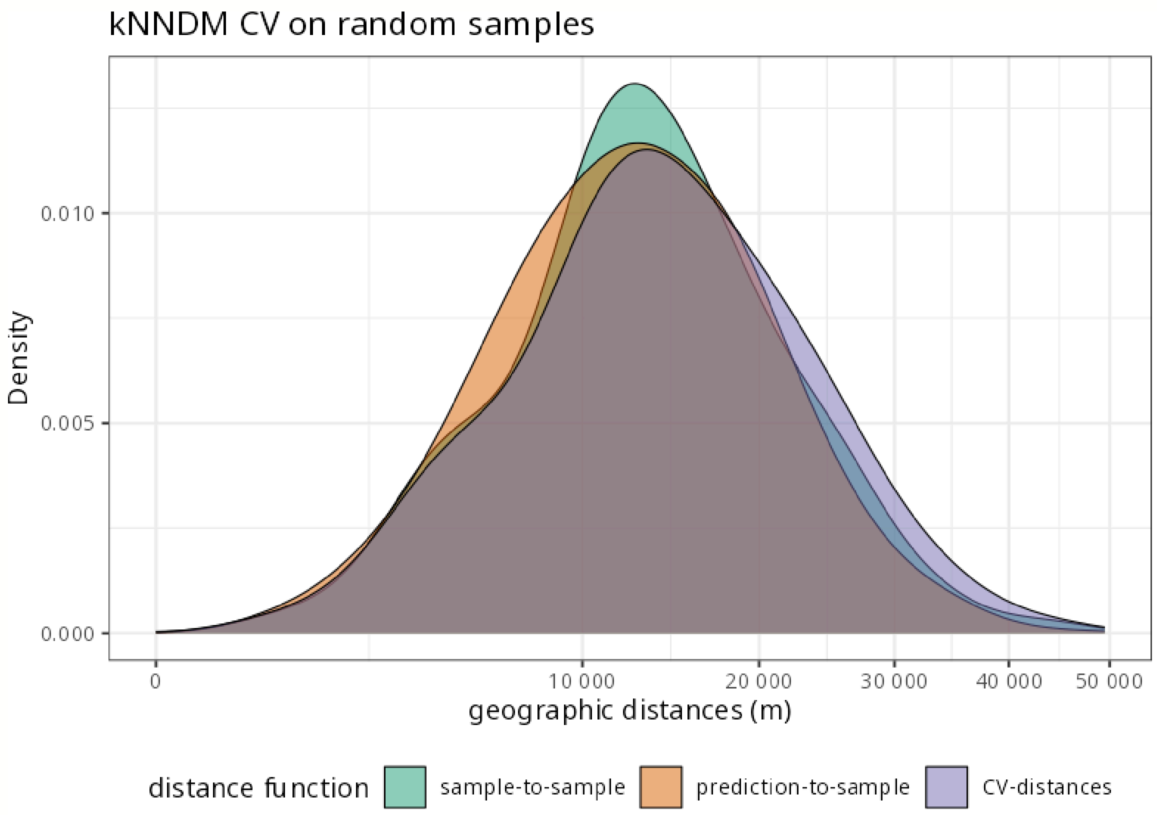





kNNDM CV fold assignments
Random
Slightly clustered
Clustered

Adaptive evaluation (kNNDM)

k-Nearest Neighbor Distance Matching ([kNNDM, Linnenbrink et al., 2024]) matches folds to the prediction scenario using distance structure (either in geographic or predictor space).



See also: NNDM, Milà et al. (2022) and DA-CV, Wang et al. (2025) for other related approaches

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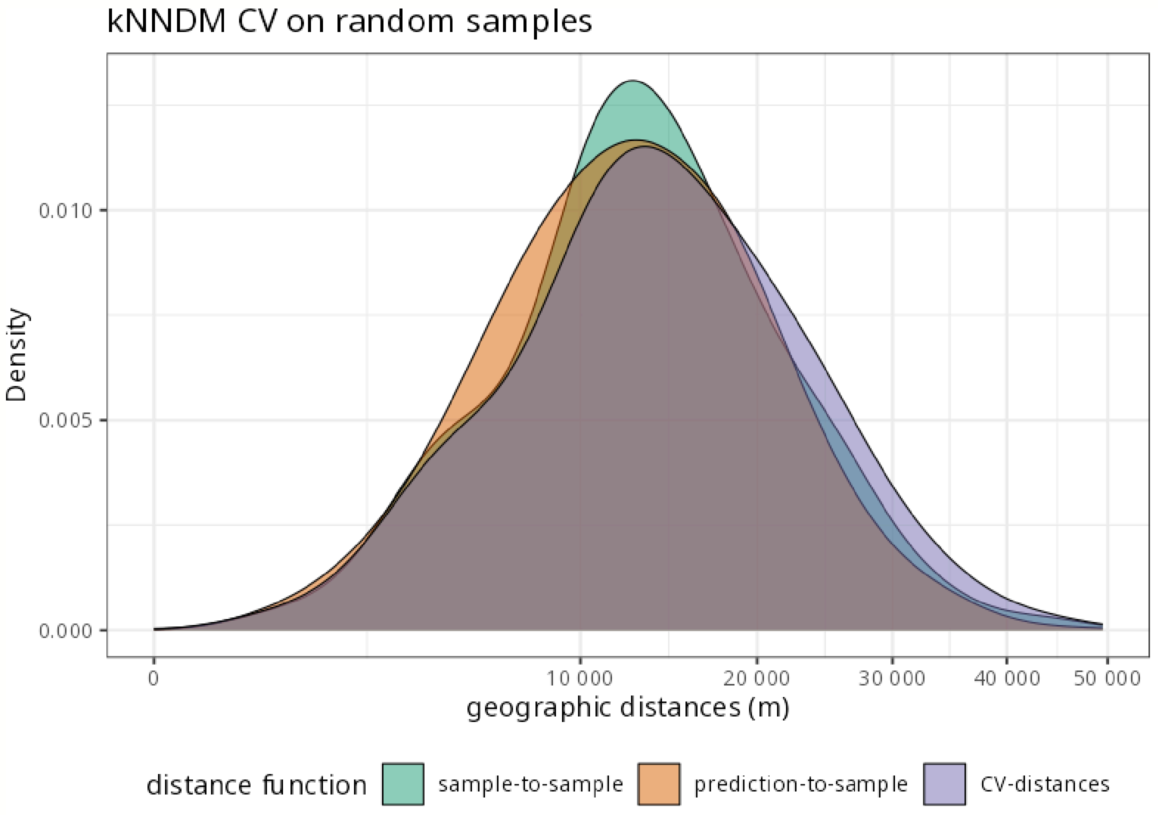

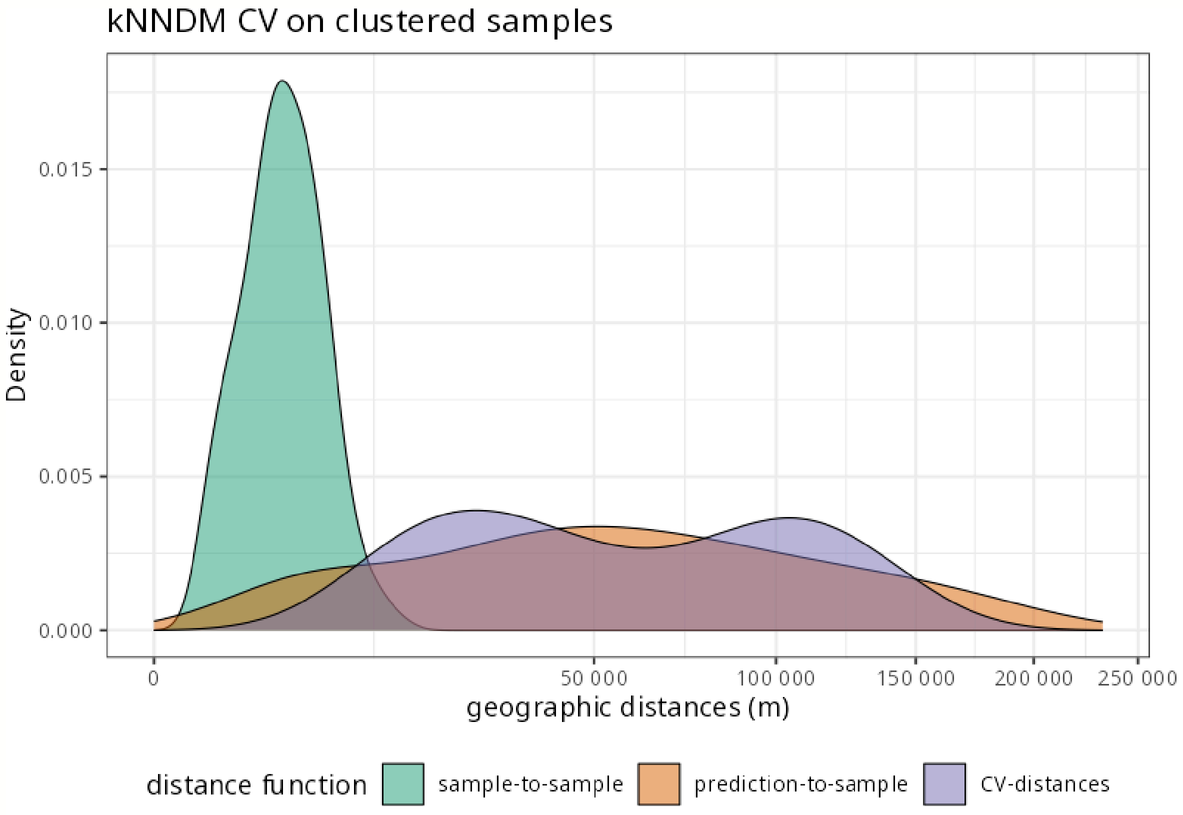

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ASSUMPTION #3

Assumptions we make

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Reality:

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All validation points are equal

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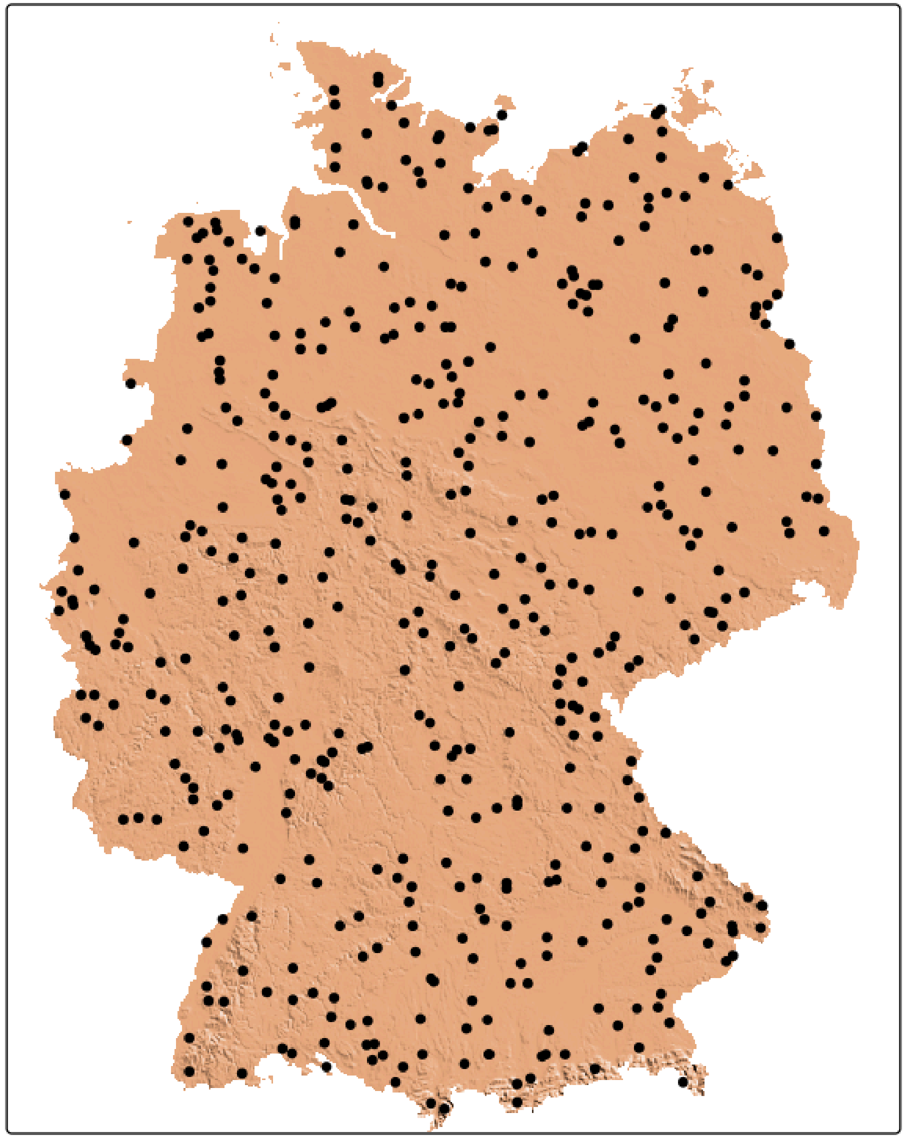
Overlapping predictor distribution(s)



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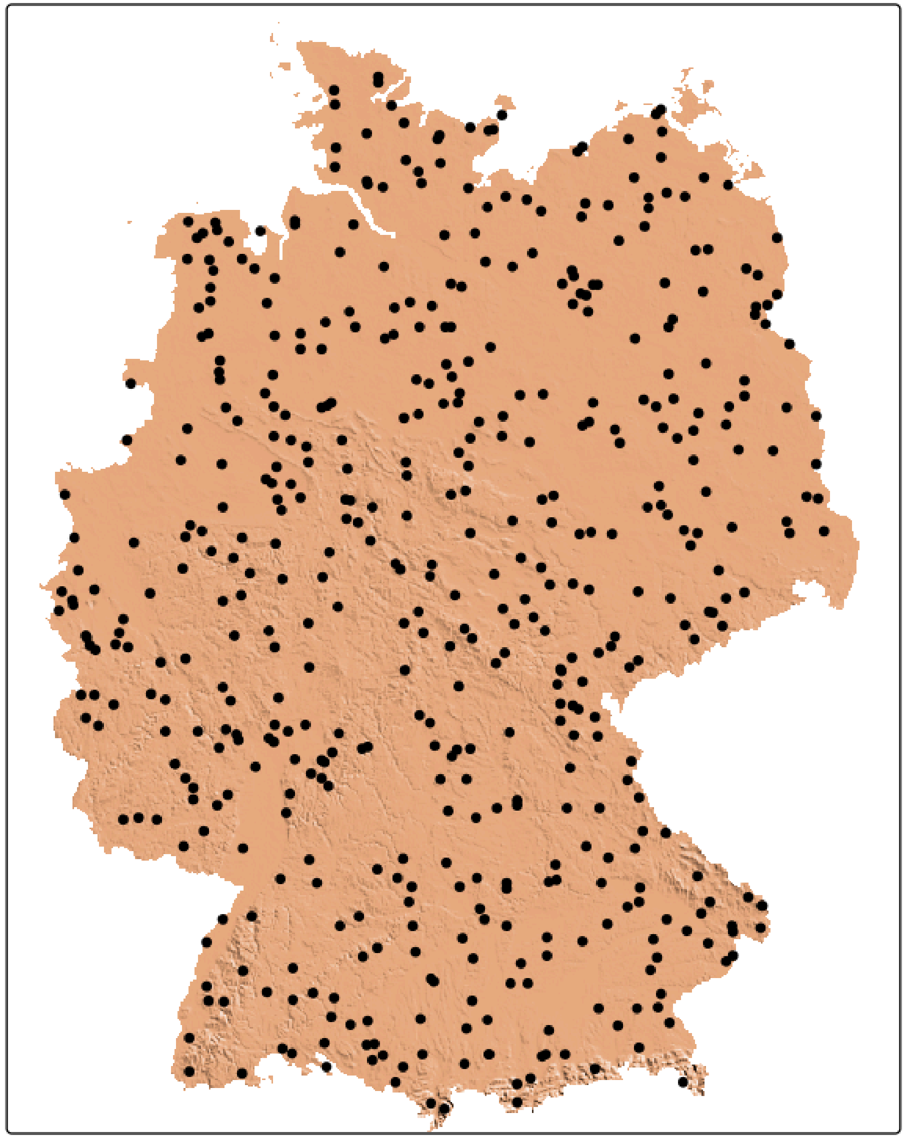
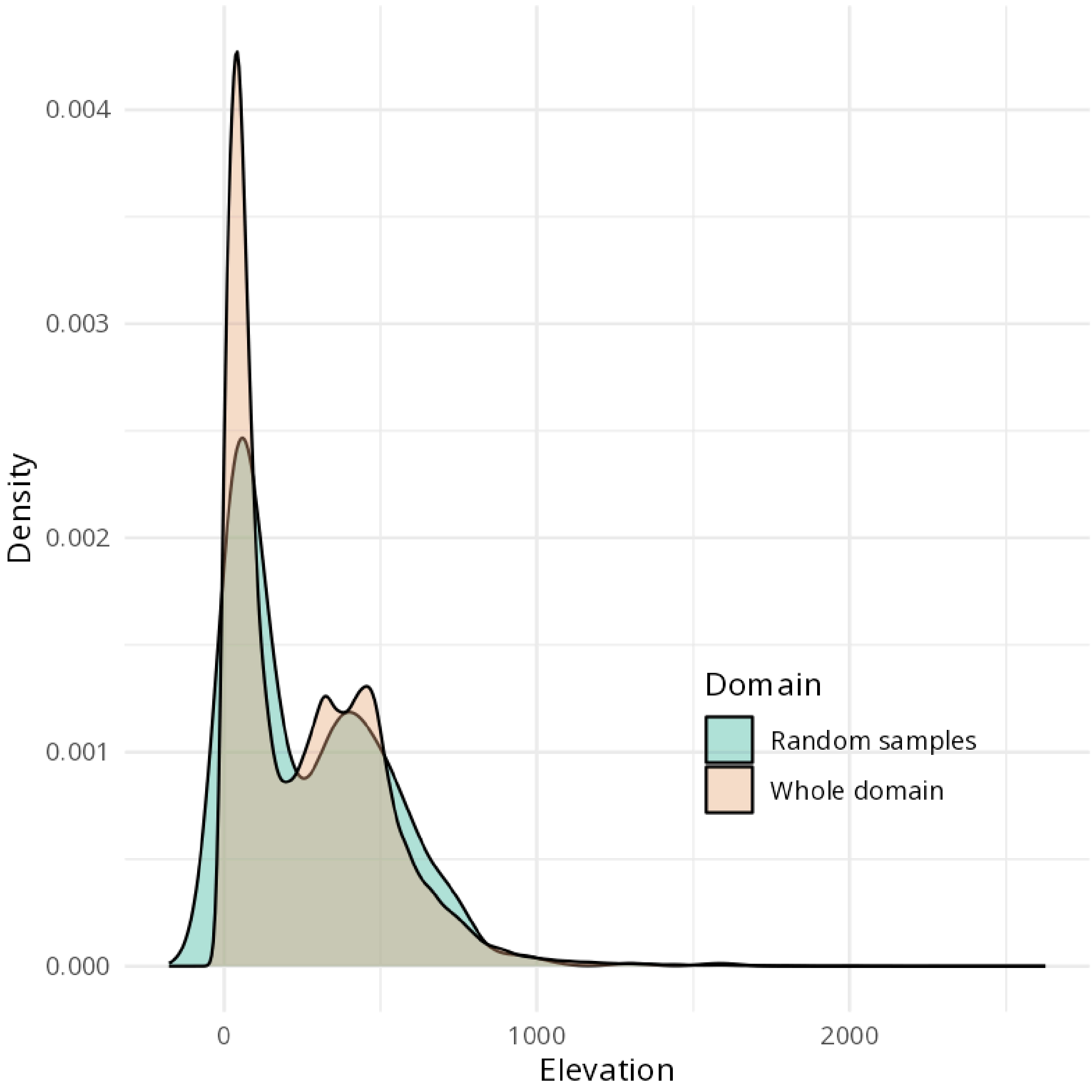
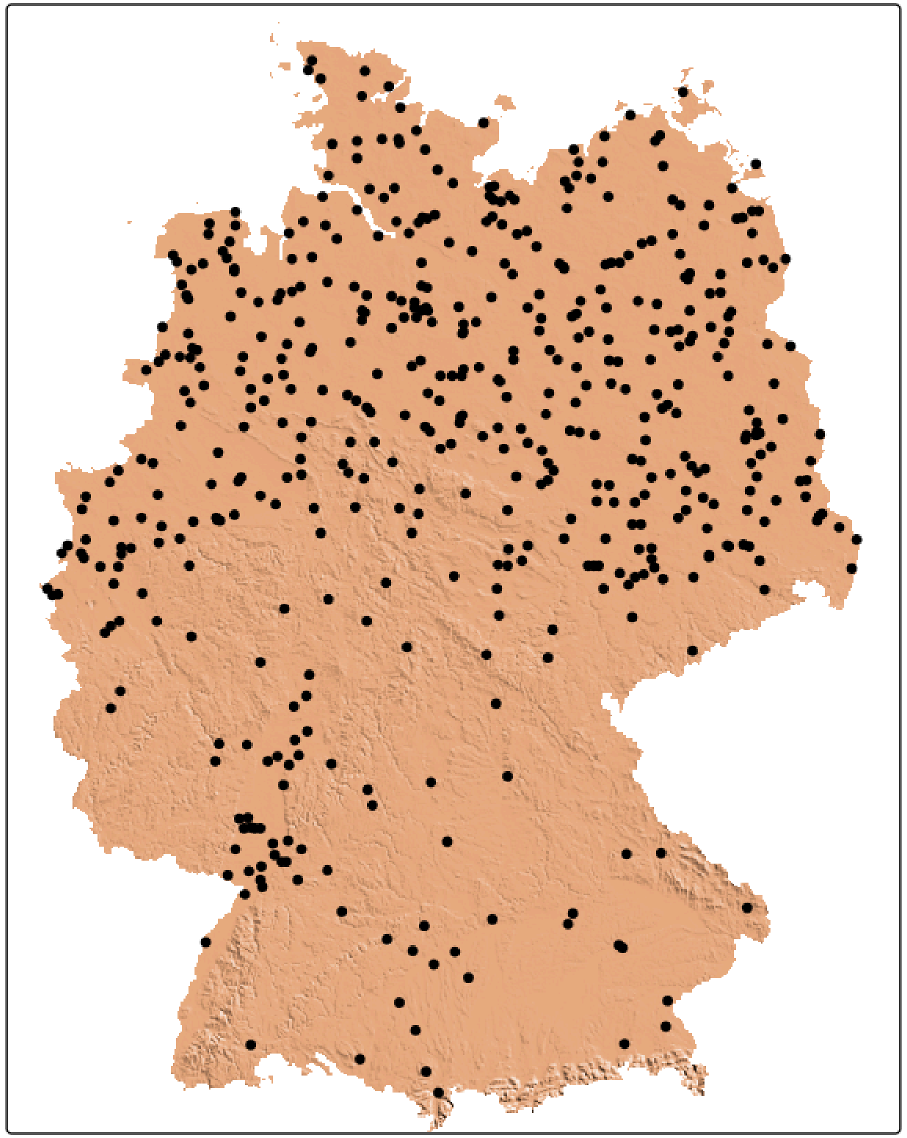
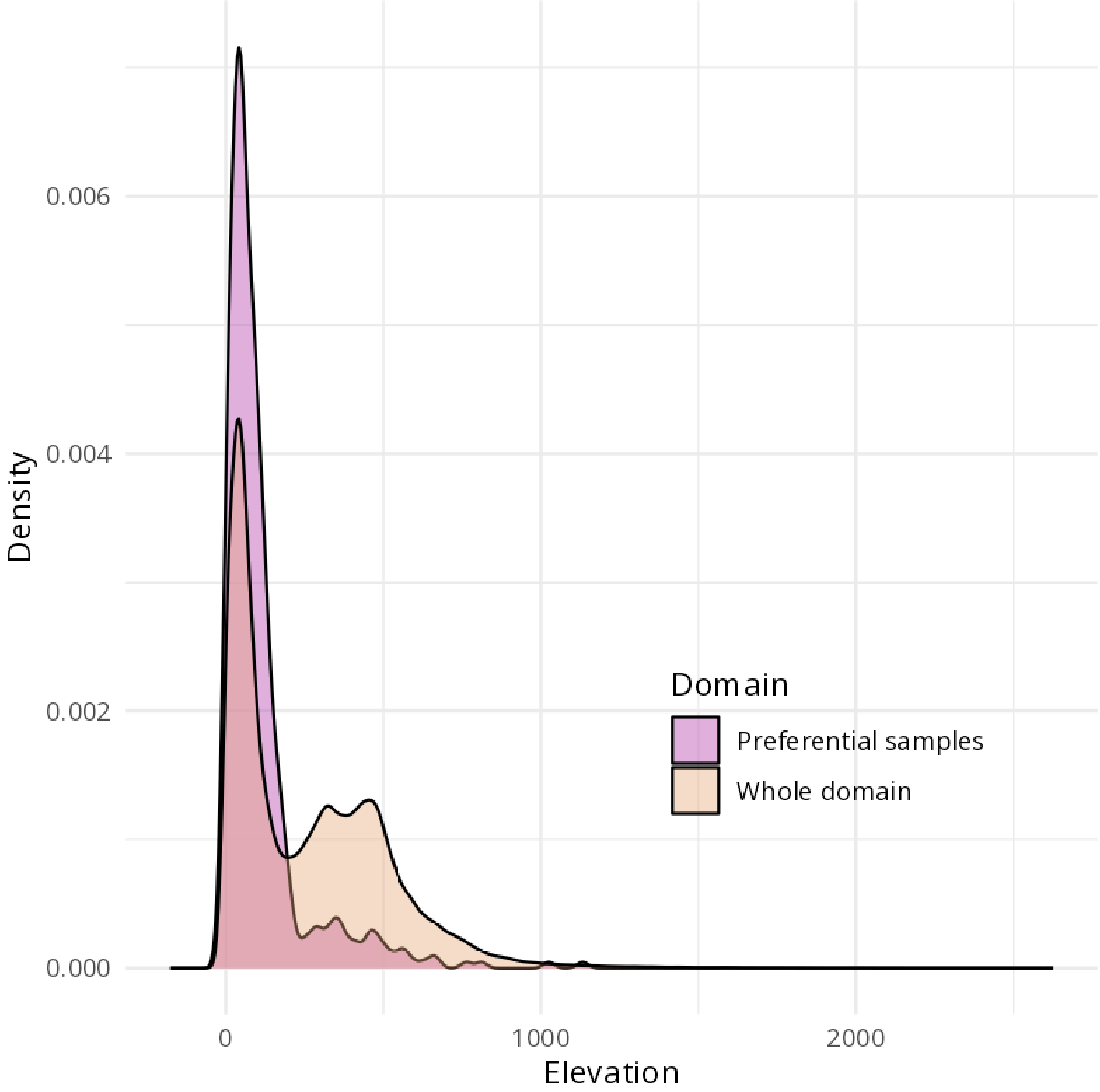




Partially overlapping predictor distribution(s)





Weighting validation points

Evaluation approach	Lowland-area weight (%)	Highland-area weight (%)	Overall RMSE
Germany domain (target distribution)	50	50	0.667

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Preferential sample (unweighted)	89	11	0.541

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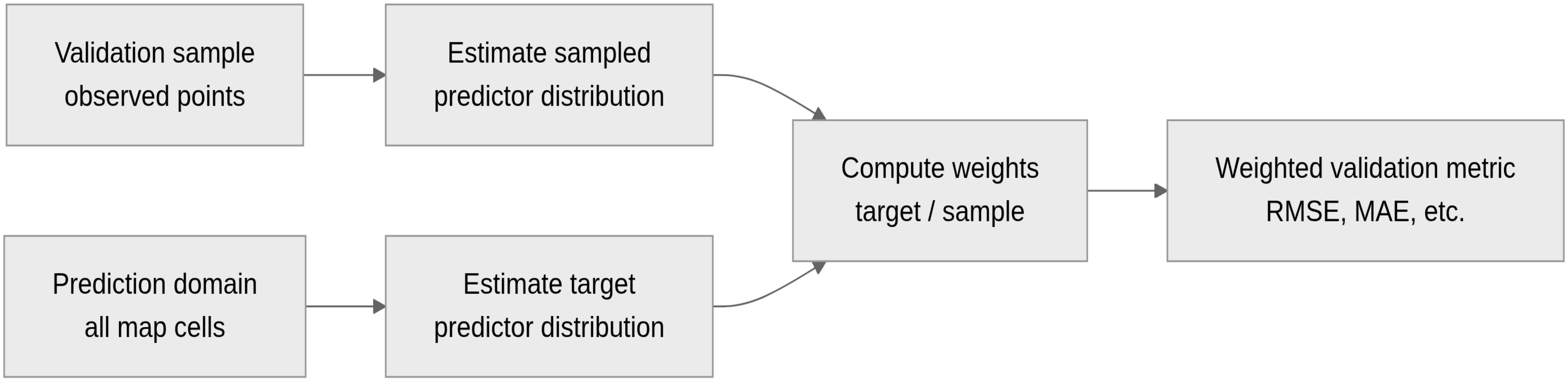
Evaluation approach	Lowland-area weight (%)	Highland-area weight (%)	Overall RMSE
Germany domain (target distribution)	50	50	0.667
Preferential sample (unweighted)	89	11	0.541
Preferential sample (reweighted)	50	50	0.667

Approaches to reweighting

Target-Weighted Cross-Validation ([TWCV, Brenning and Suesse, 2026]) adjusts cross-validation weights to align evaluation with the prediction domain rather than the sampled data distribution.



From assumptions to results

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~~There is one "correct" validation approach~~

Reality:

The validation strategy should follow the prediction task.

~~All validation points are equal~~

Reality:

Prediction conditions are not equally common.

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Possible solution: identify regions of reliable prediction.

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Possible solution: use adaptive evaluation strategies to create folds that resemble the prediction scenario.

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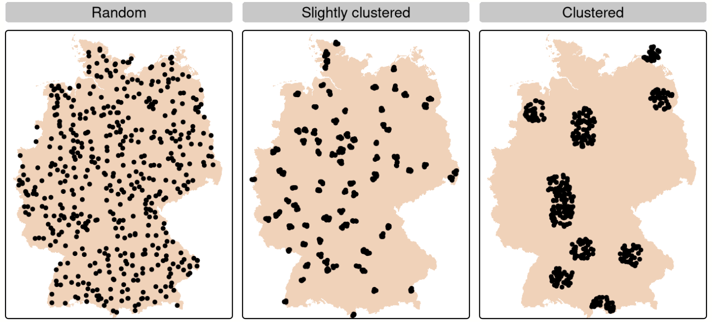
Reality:

Prediction conditions are not equally common.

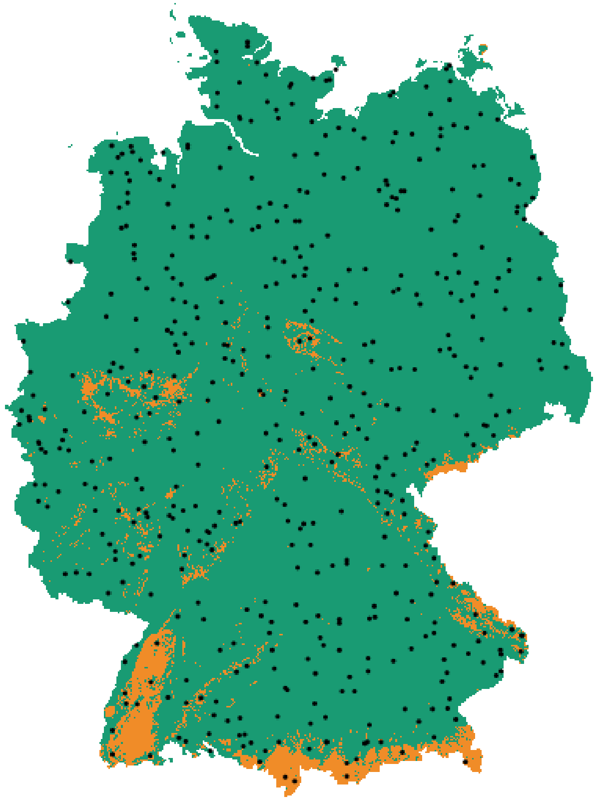
Possible solution: weight validation points according to their prevalence in the prediction area.

A piece of evidence

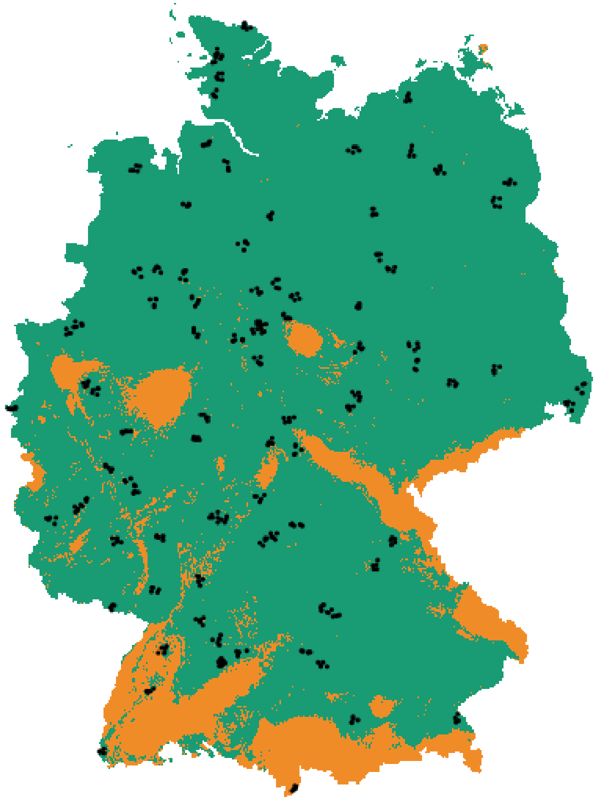
Area of applicability for different sampling designs



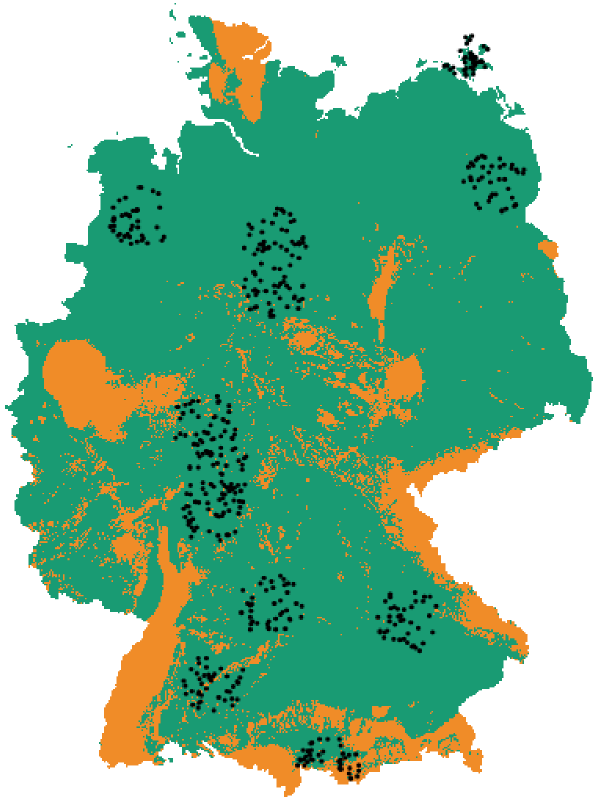
Random samples (93.9% inside AOA)



Slightly clustered samples (85.7% inside AOA)

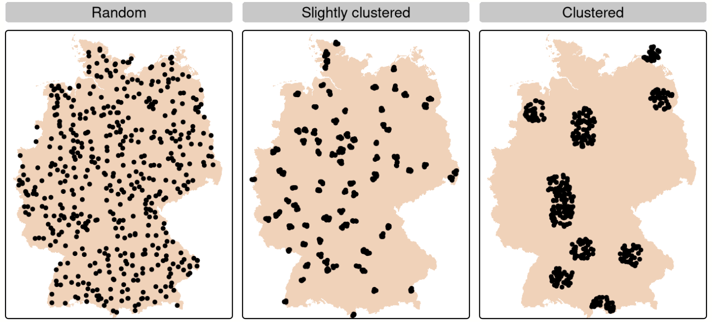


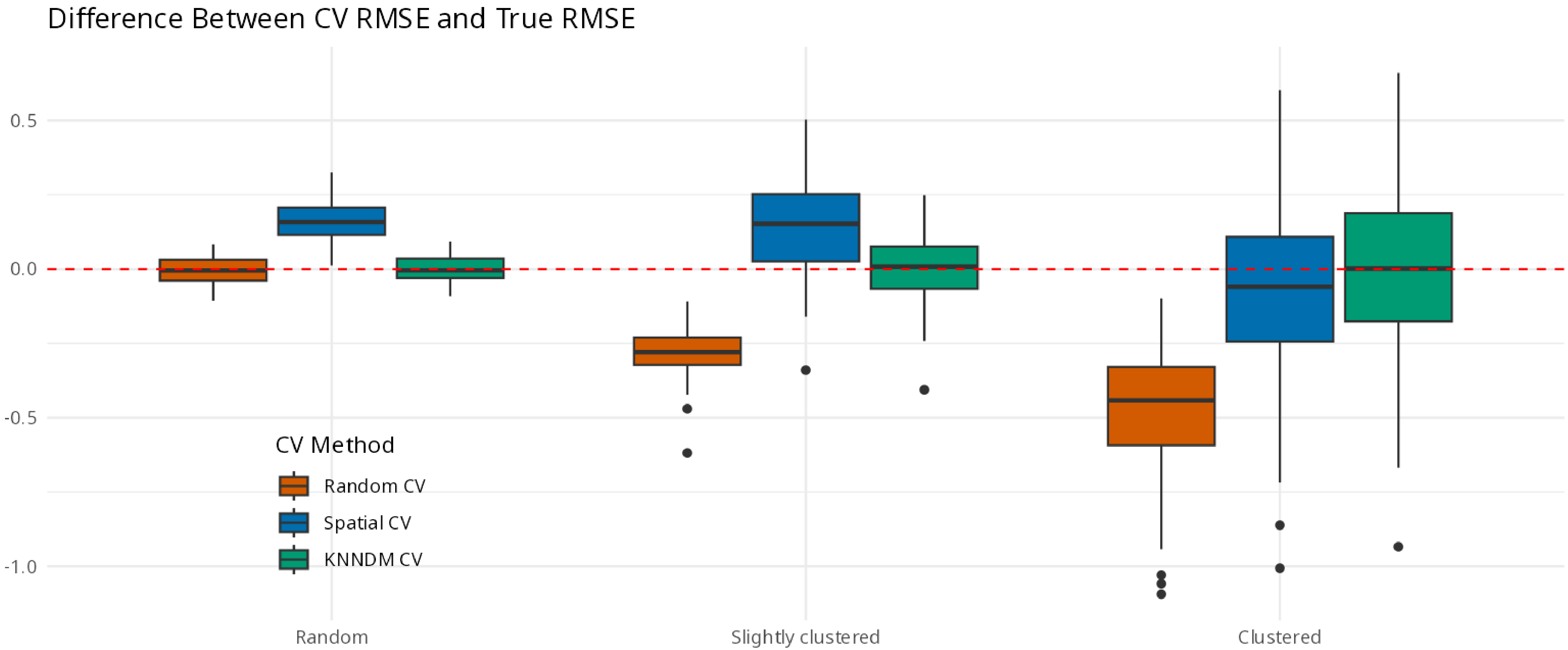
Clustered samples (81.8% inside AOA)



A piece of evidence

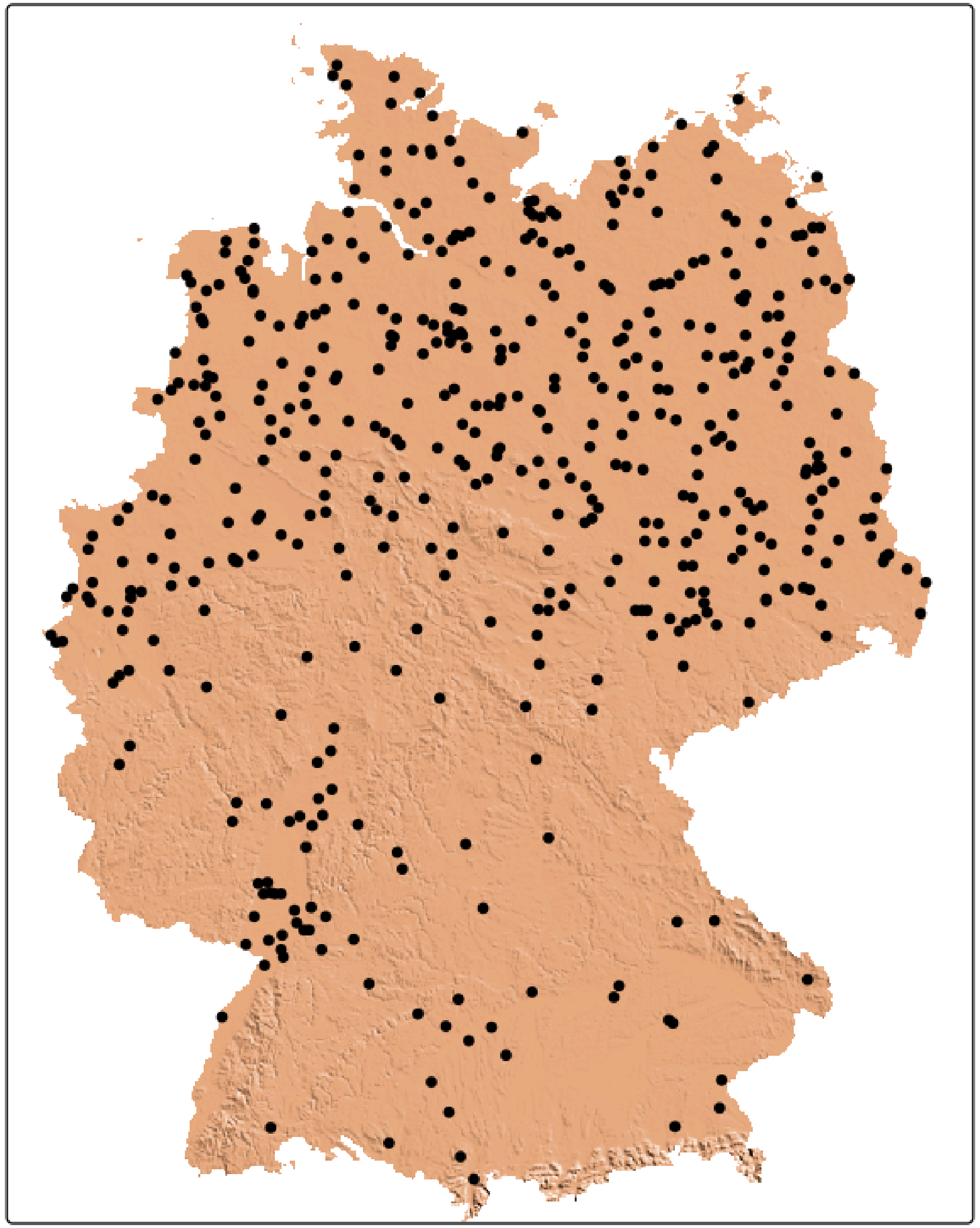
Evaluation results for different validation strategies

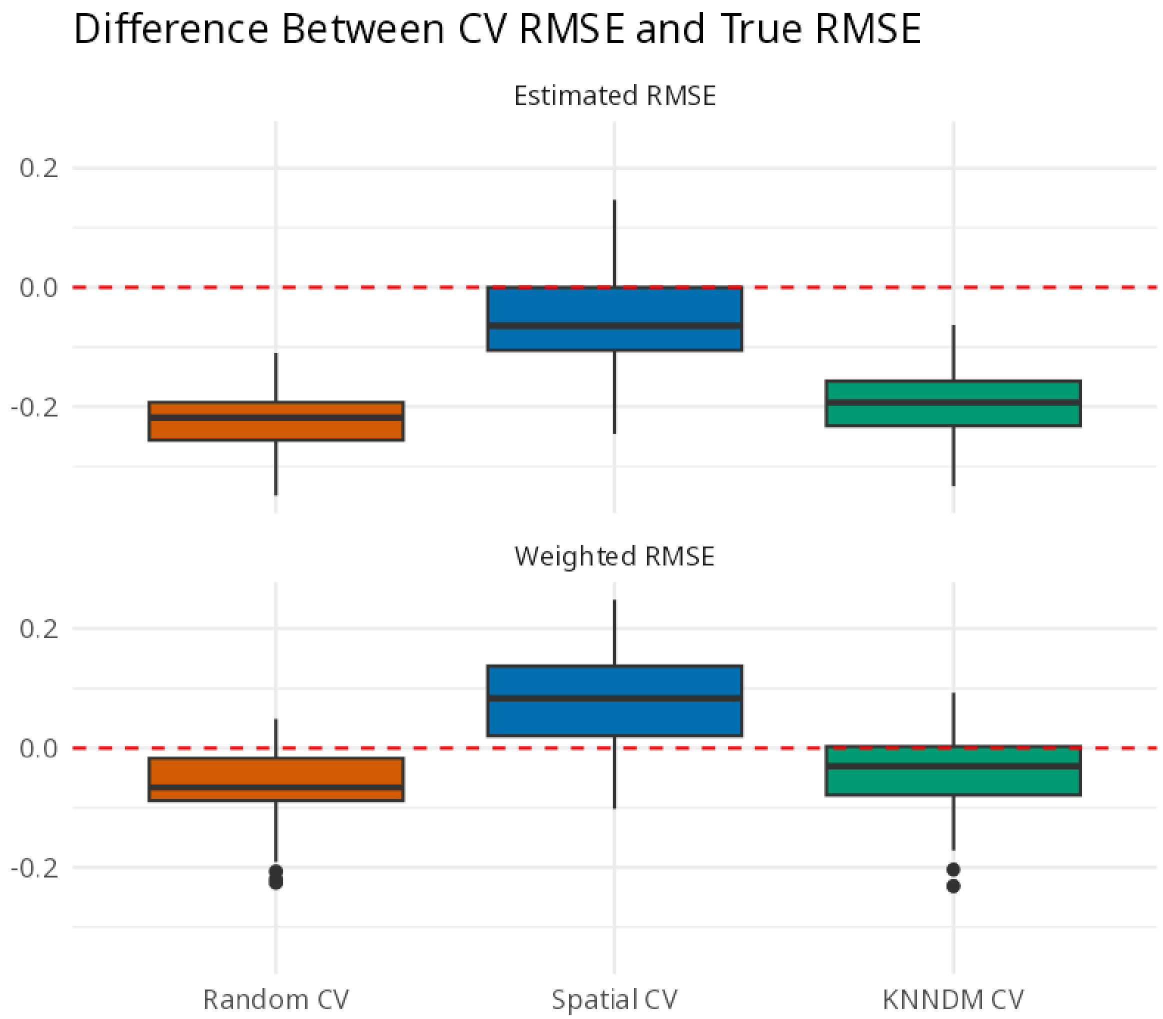




A piece of evidence

Effect of weighting validation points





Key components of *prediction-domain adaptive evaluation*

Contact

https://jakubnowosad.com

Resources

Papers: Nowosad et al., 2026,
Linnenbrink et al., 2026

Slides:

Acknowledgements

Remote Sensing & Spatial Modelling

Machine Learning for Earth Observation
22 - 24th June 2026

Funded by the European Union

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Key components of *prediction-domain adaptive evaluation*

1. **Define the prediction domain**
2. **Construct validation folds that reflect the prediction domain**
3. **Weight validation samples by their prevalence in the prediction domain**

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https://jakubnowosad.com

Resources

Papers: Nowosad et al., 2026, Linnenbrink et al., 2026

Slides:

Acknowledgements

Remote Sensing & Spatial Modelling

Machine Learning for Earth Observation
22 - 24th June 2026

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Key components of *prediction-domain adaptive evaluation*

1. **Define the prediction domain**
2. **Construct validation folds that reflect the prediction domain**
3. **Weight validation samples by their prevalence in the prediction domain**

Open questions remain, including how to mix these three components together.

Also: these are three important components, not a complete theory of spatial ML evaluation.

Contact

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