

Predicting into unknown space?

Estimating the area of applicability of spatial prediction models

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1 Institute of Landscape Ecology, WWU Münster

2 Institute for Geoinformatics, WWU Münster

Problem: Moving from field observations to maps of ecosystem variables



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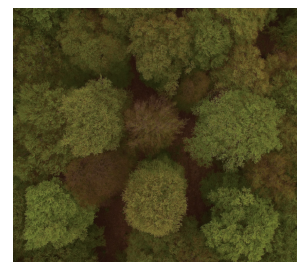
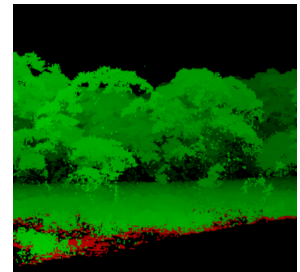
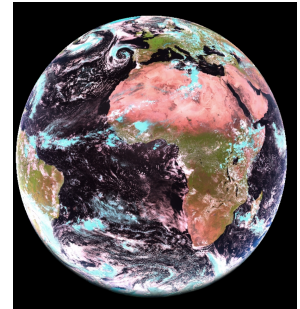
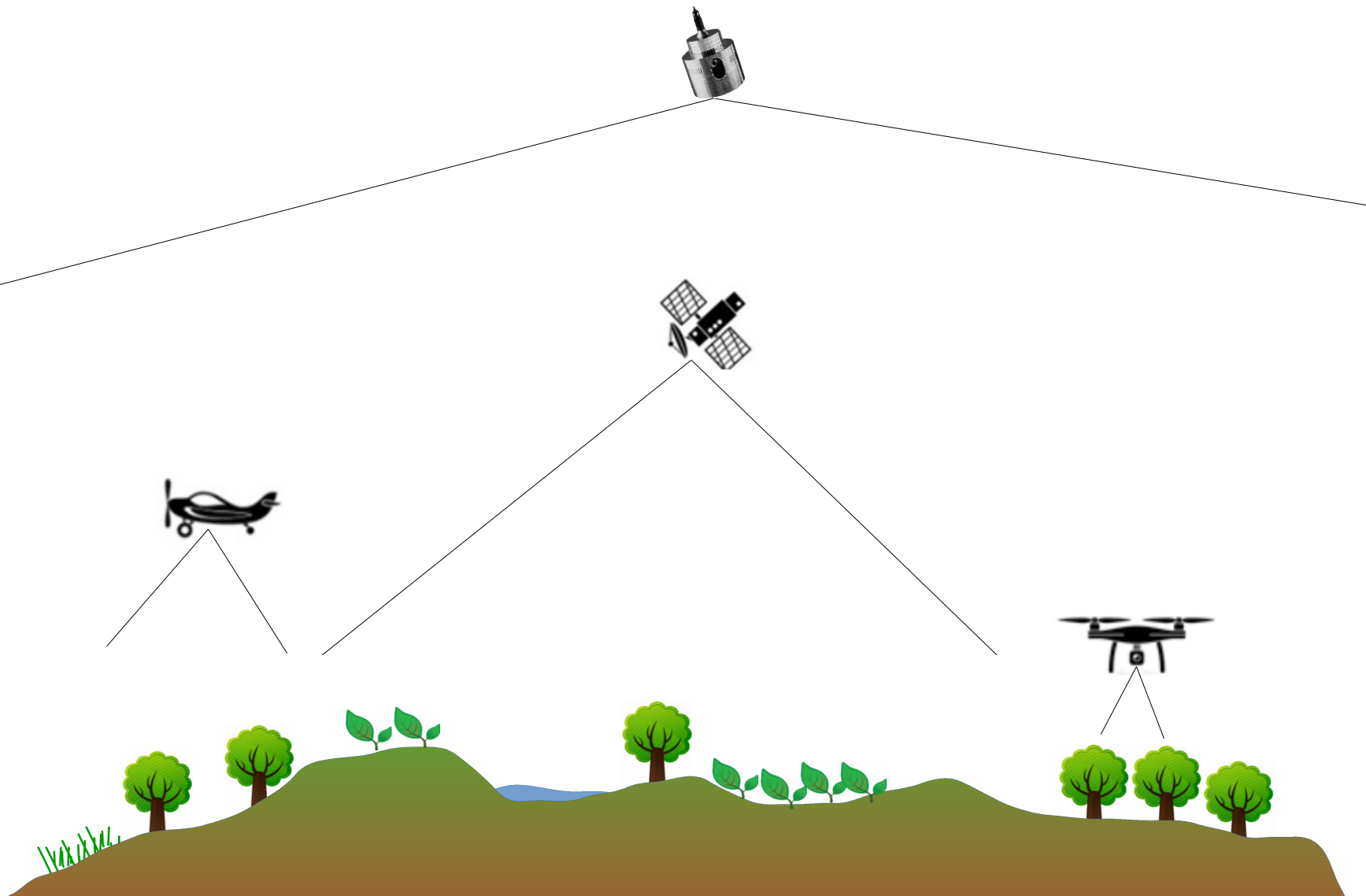


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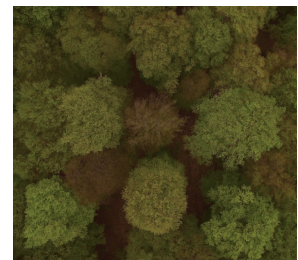
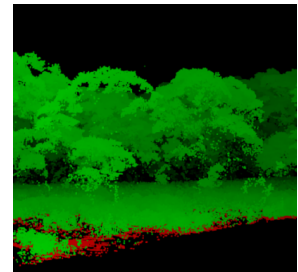
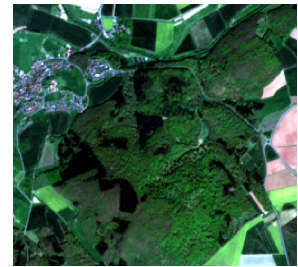
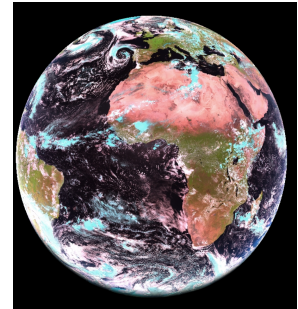
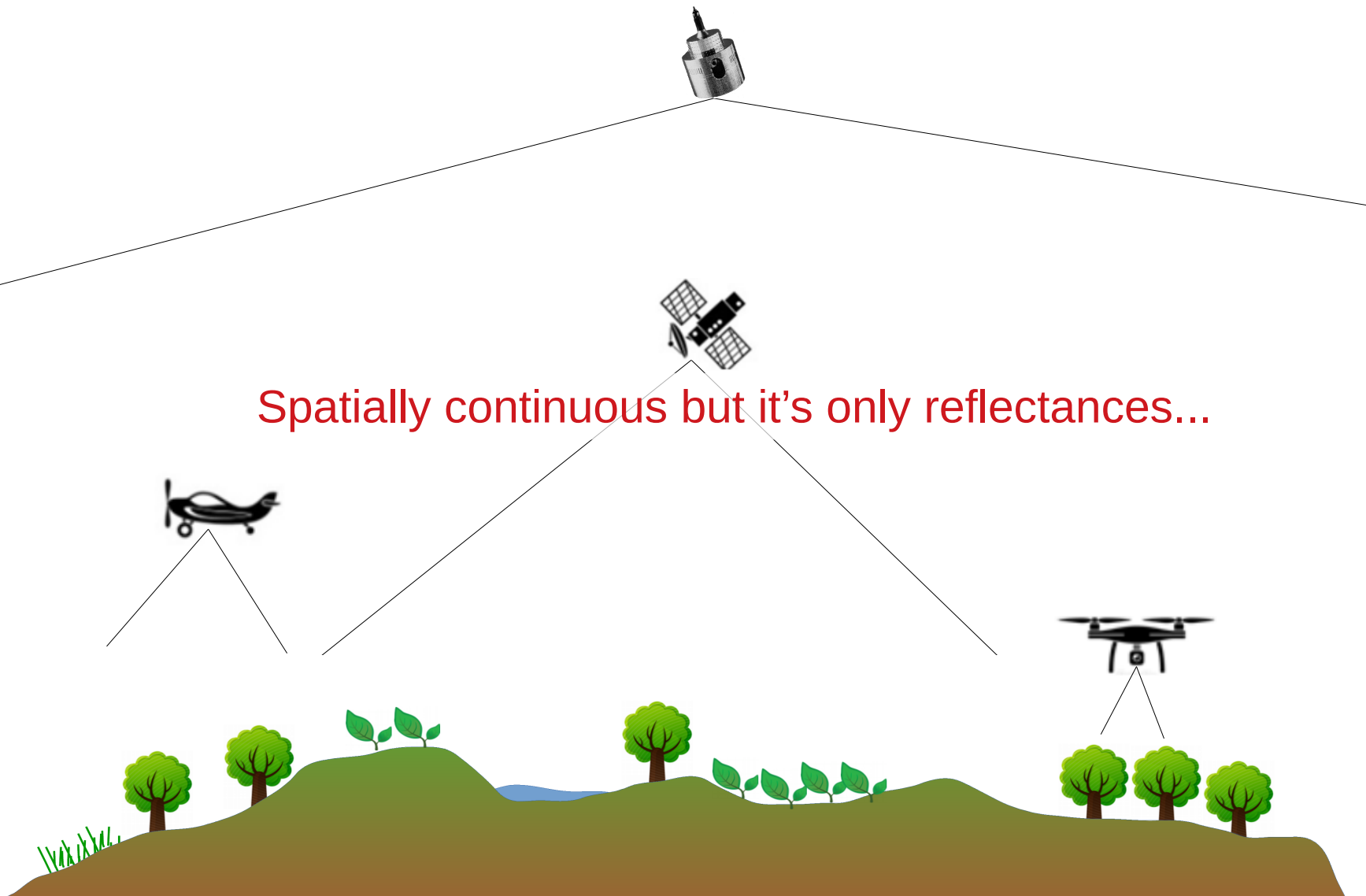


How do we fill the gaps between sampling locations?

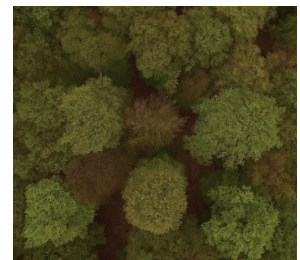
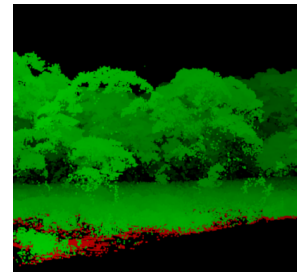
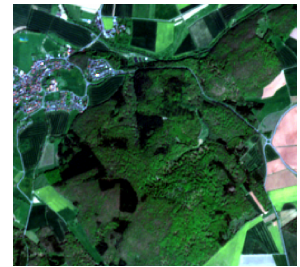
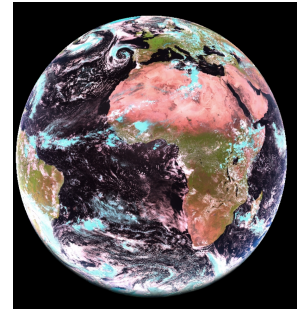
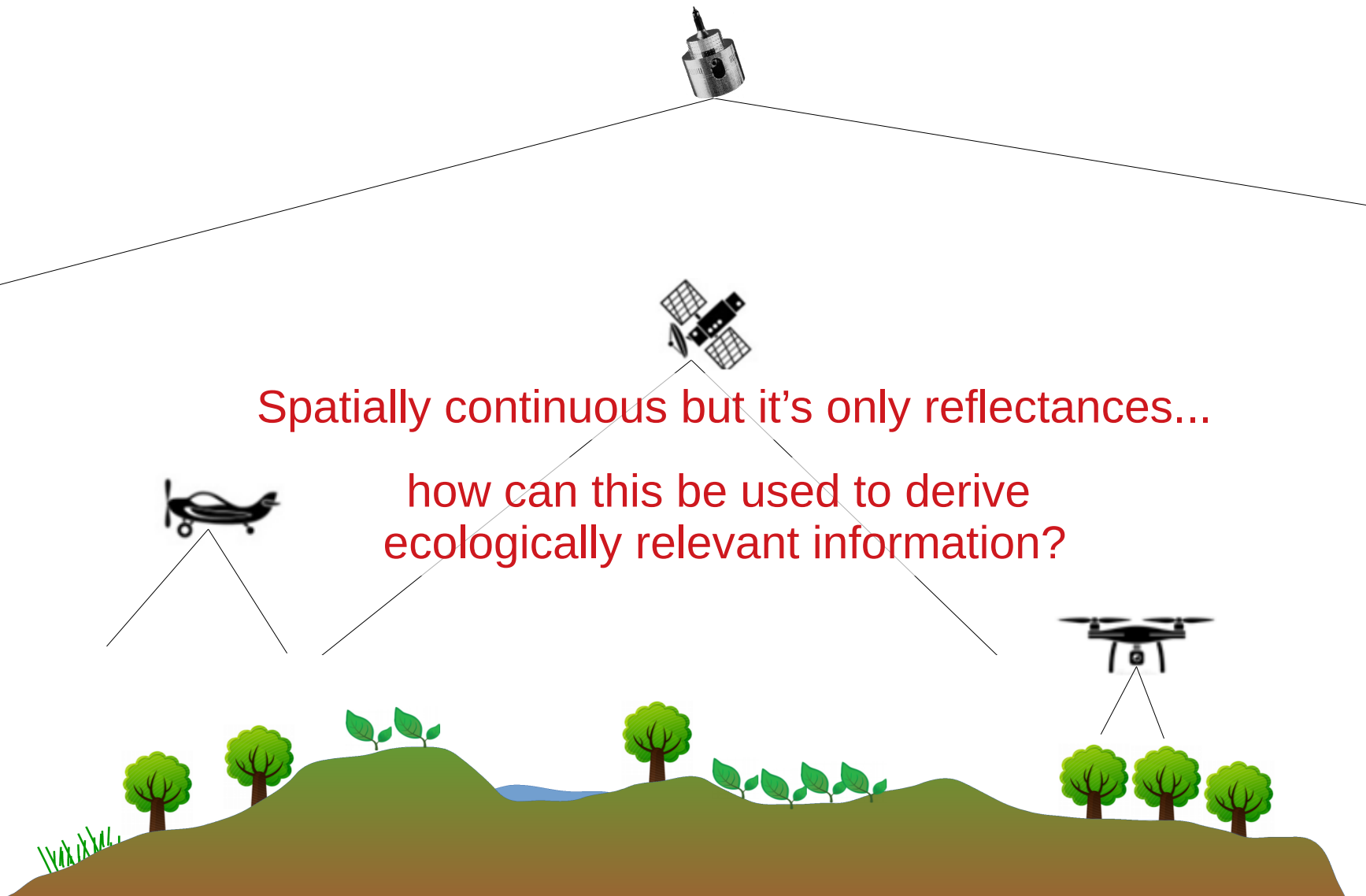
Remote Sensing of landscapes



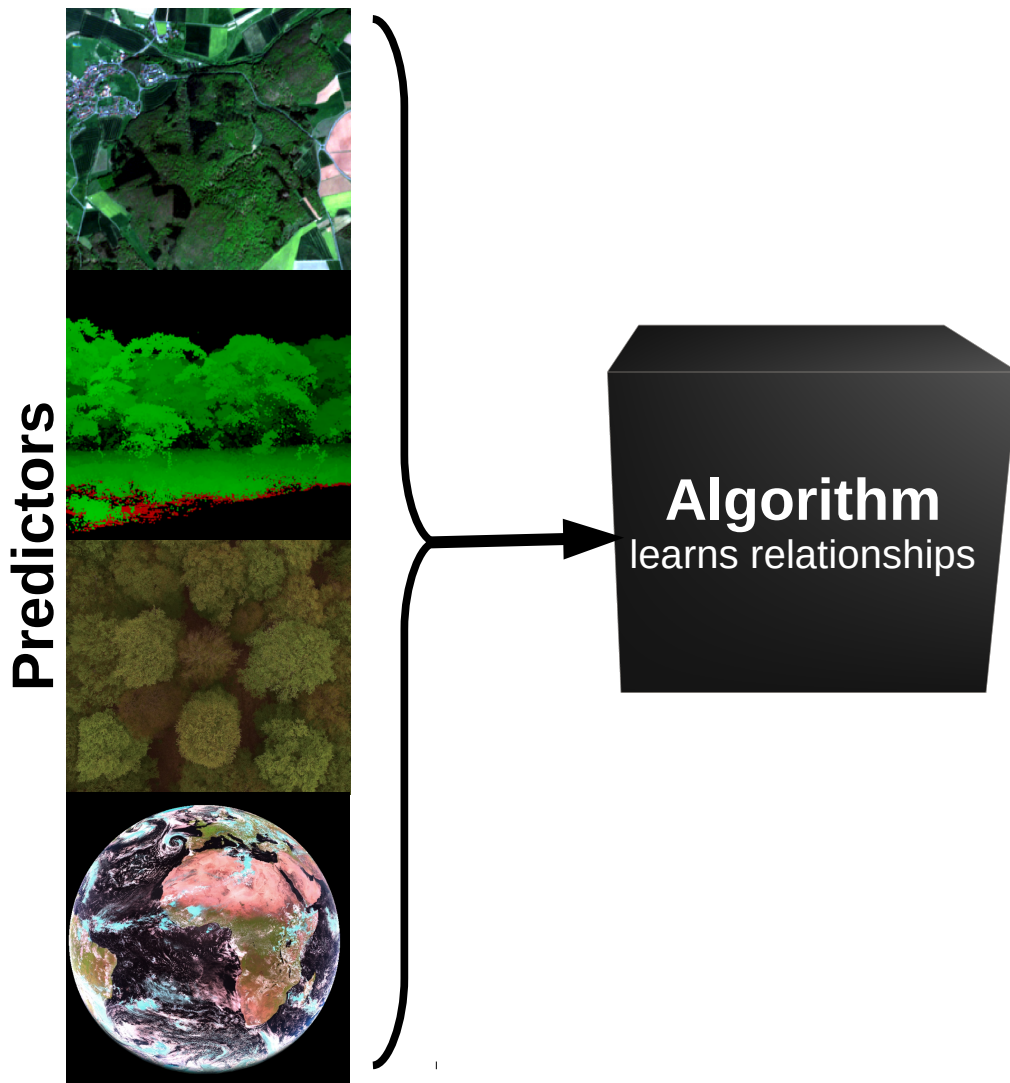
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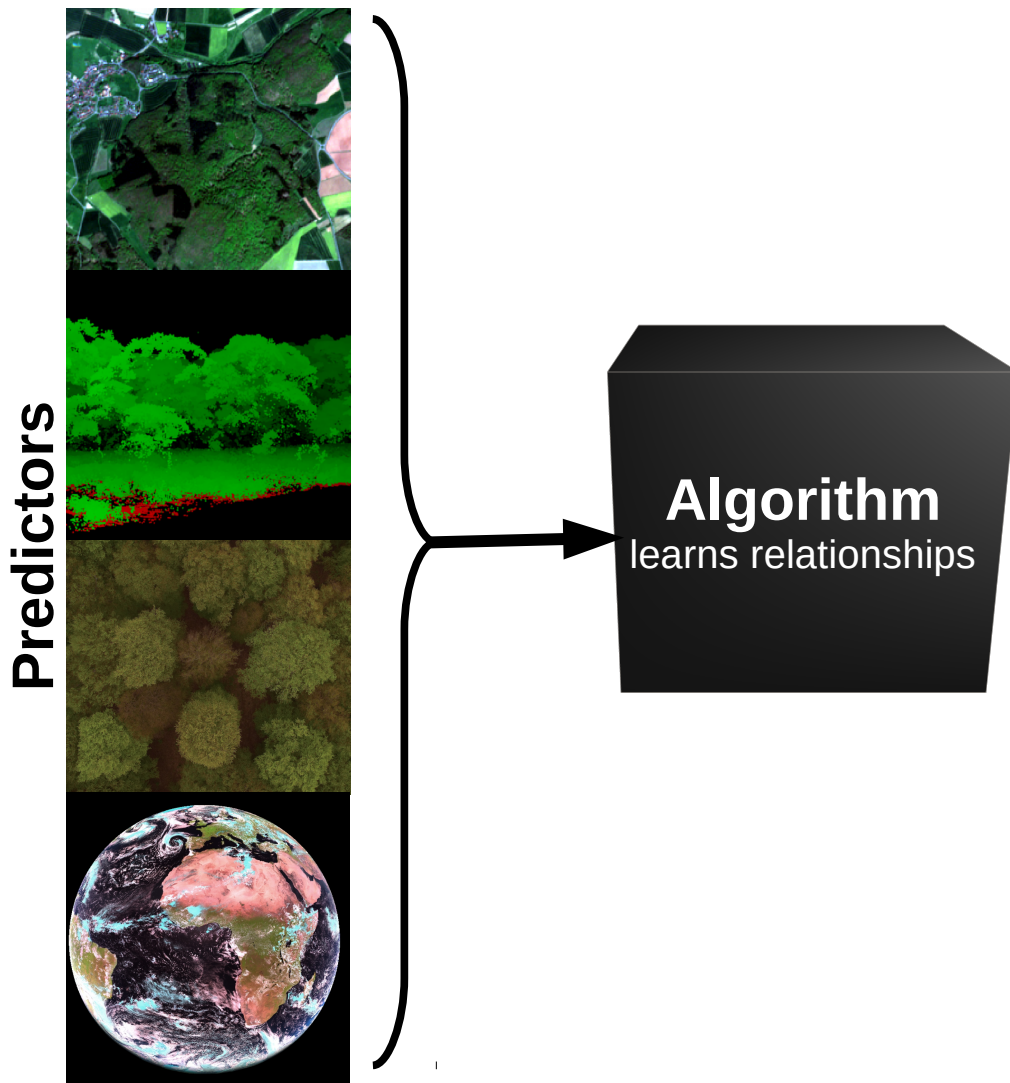
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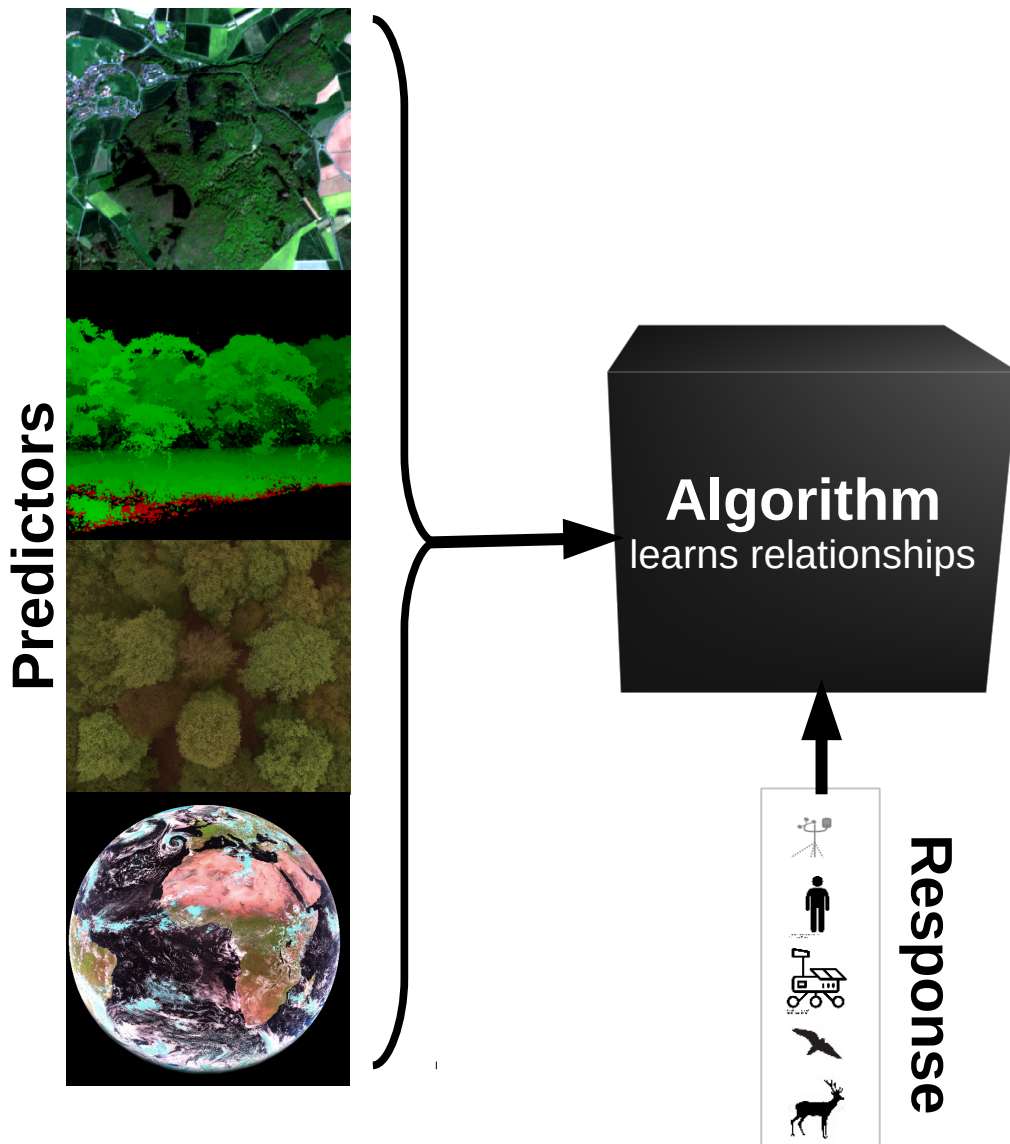
Predictive modelling of the environment: The machine learning way



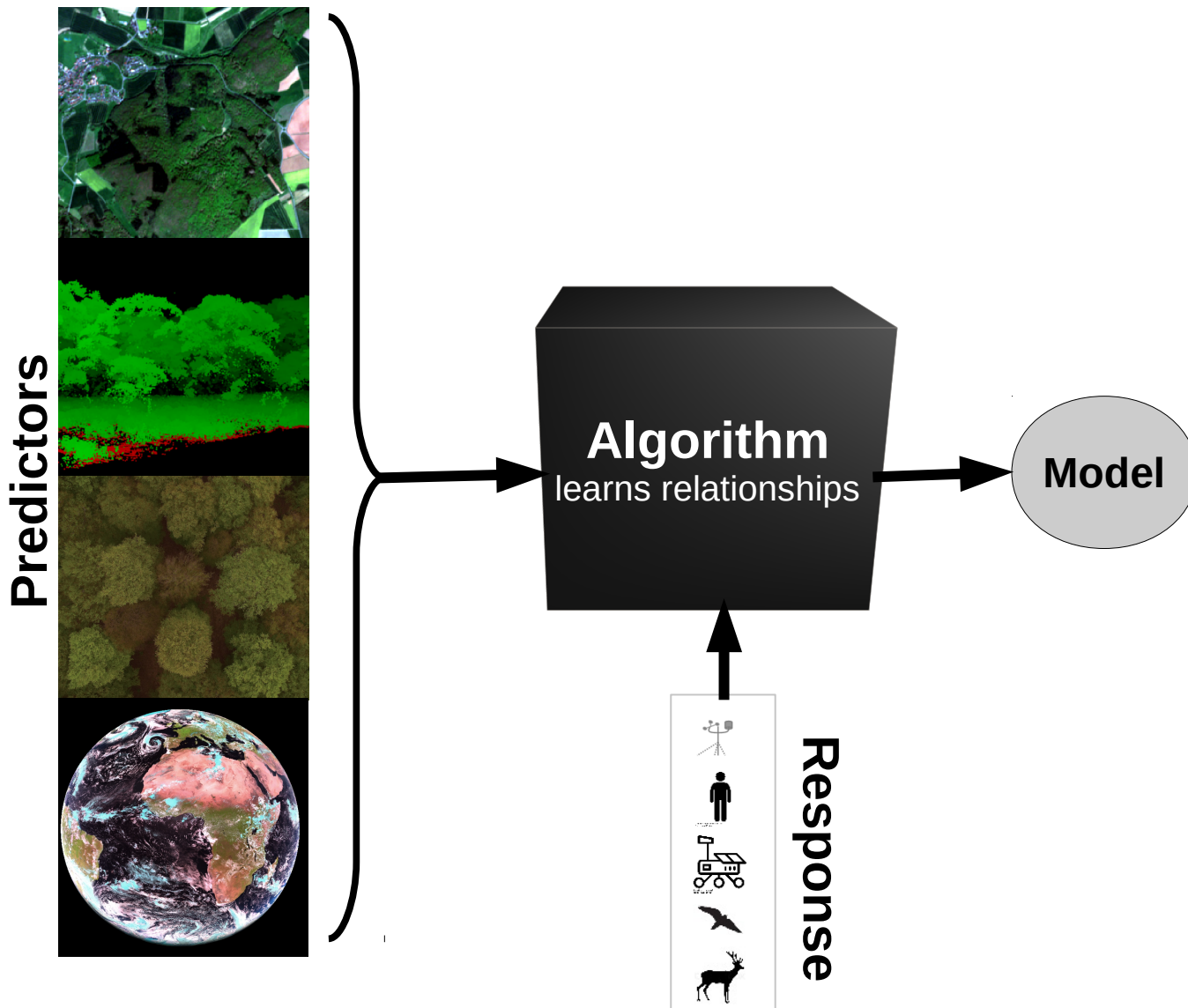
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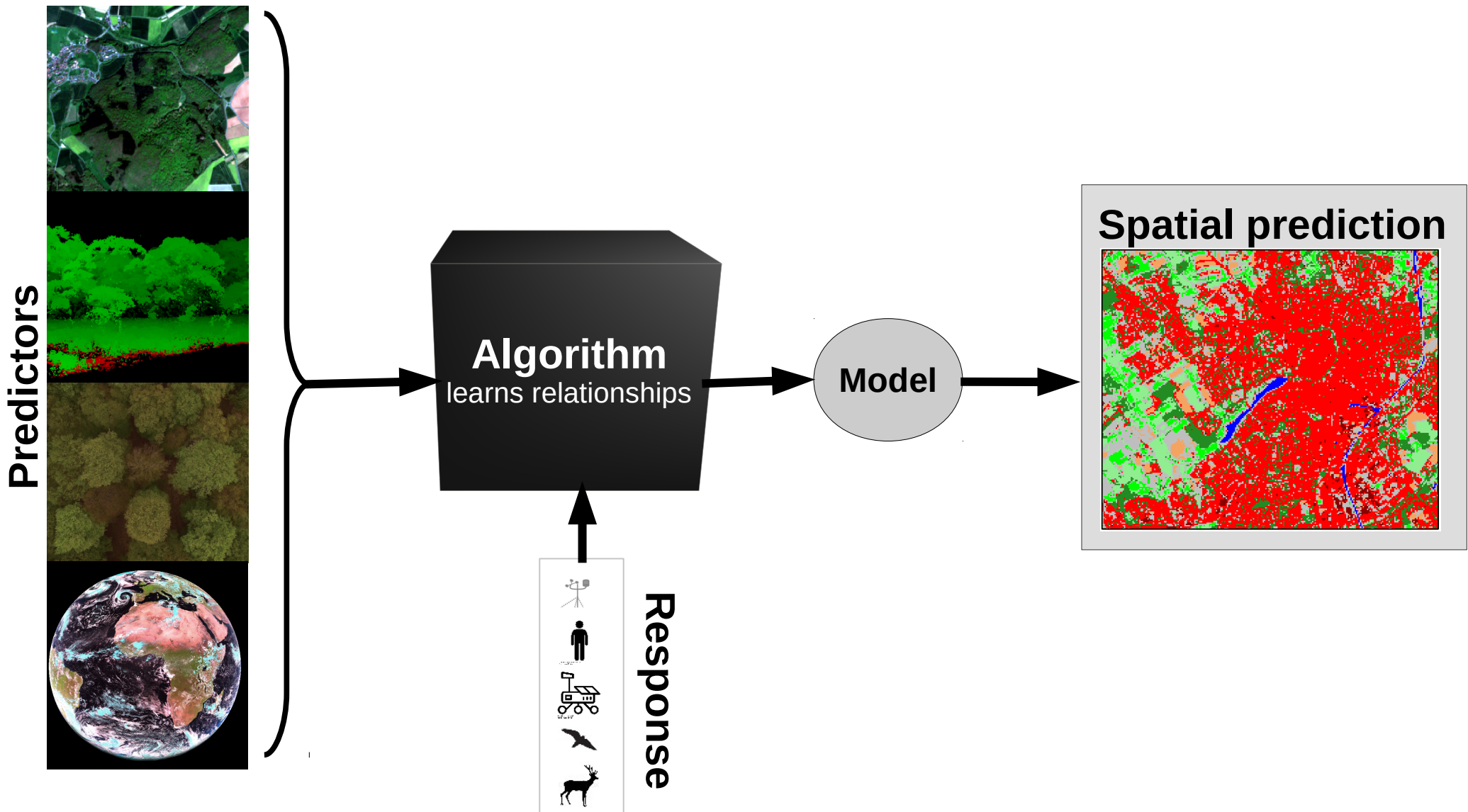
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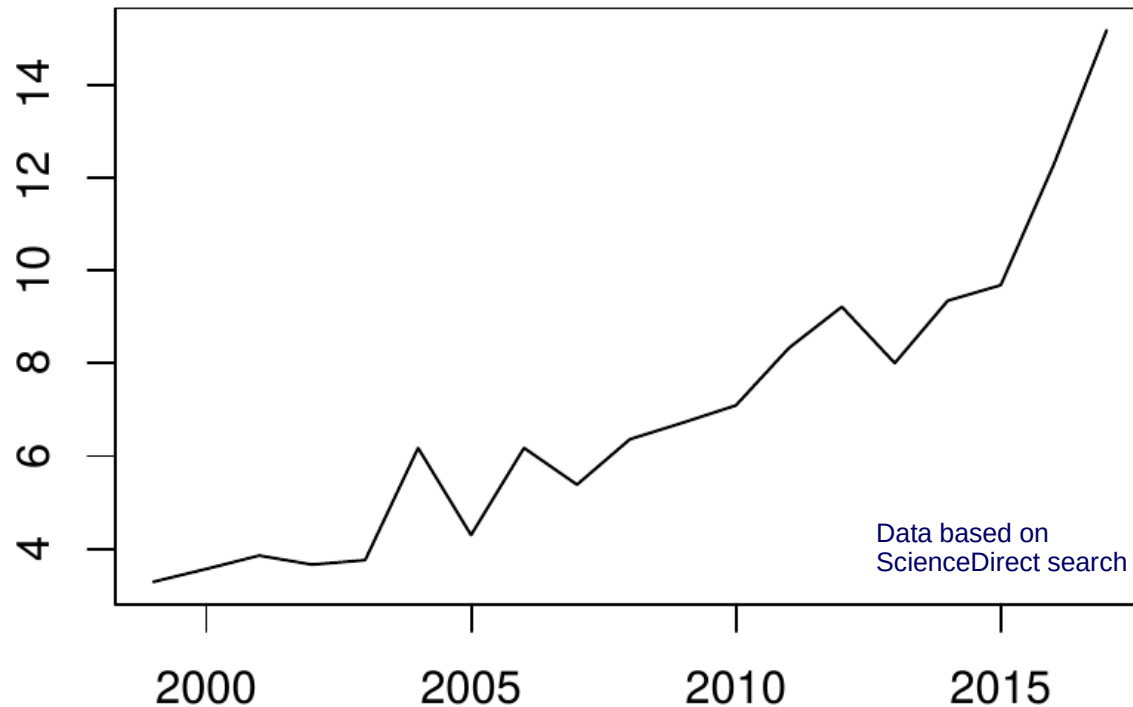


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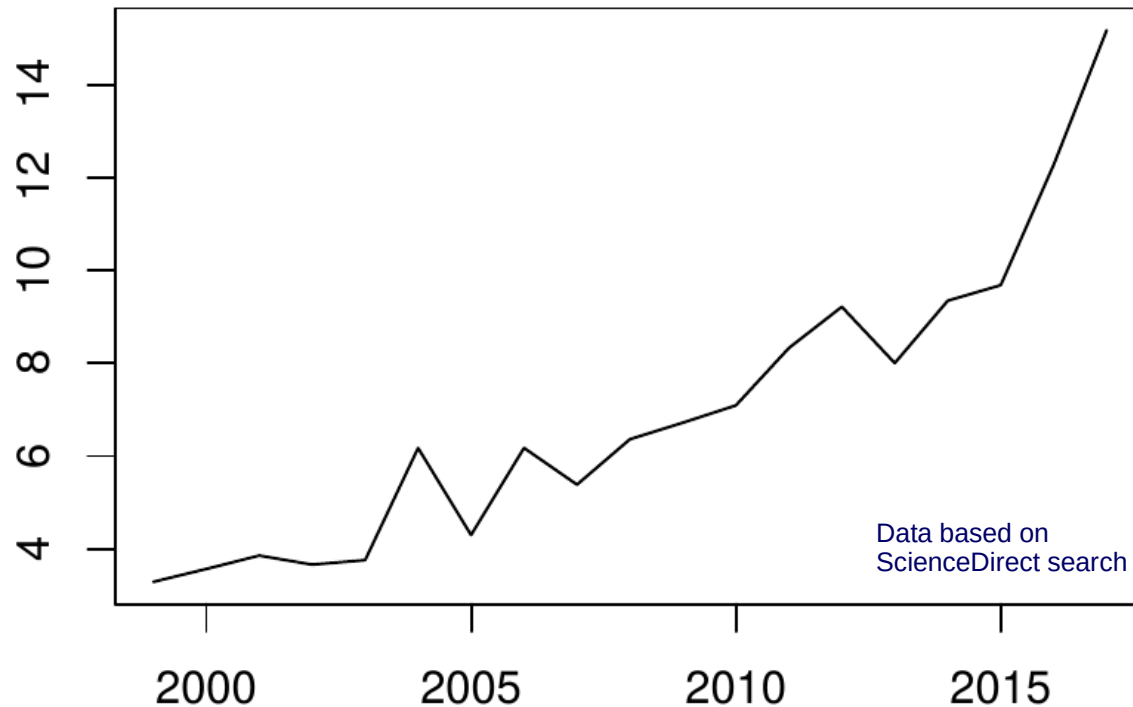
Global maps of ecosystem variables based on machine learning

Proportion of publications that use machine learning in environmental remote sensing



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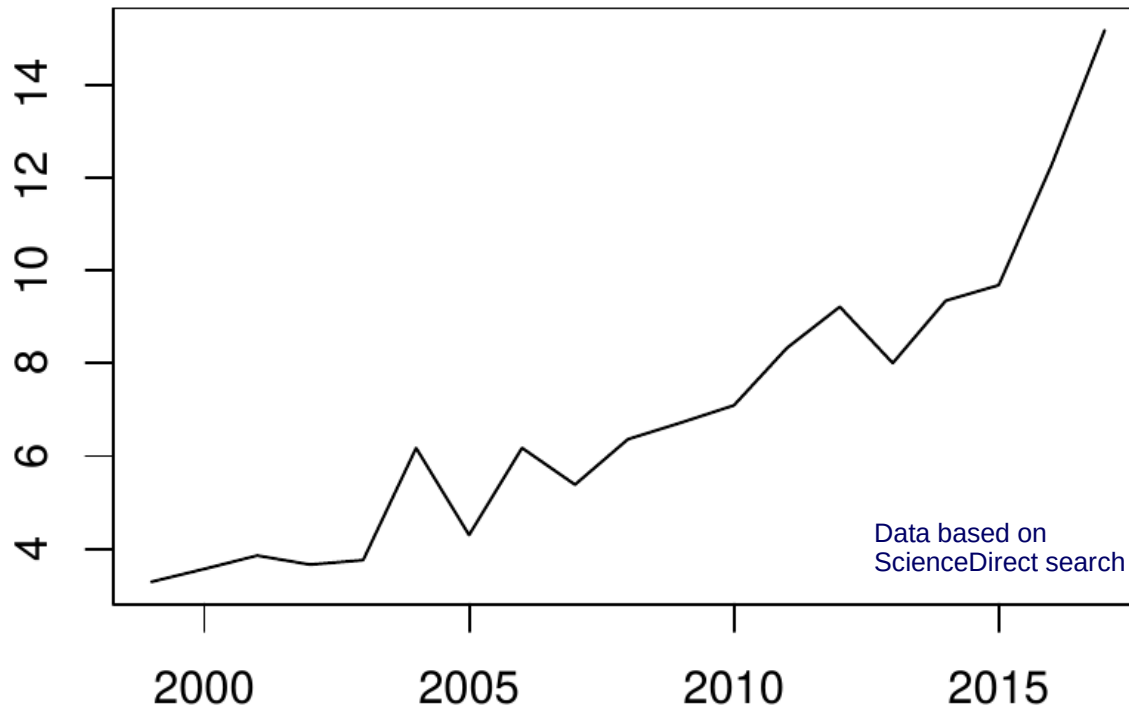


Including **global** datasets on

- soil properties
- abundances of microorganisms
- Biodiversity
- tree restoration potential
- ...and many more

Global maps of ecosystem variables based on machine learning

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- soil properties
- abundances of microorganisms
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- tree restoration potential
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Machine learning as a „magic tool“ to map basically everything ?

...but there are increasingly doubts about the methods

Wissenschaft

Wenn die KI daneben liegt

Welche Fehler drohen, wenn Forscher Wissenslücken per Computer schließen wollen, zeigen zwei aktuelle Klimastudien.

Von **Tin Fischer**

6. November 2019, 16:44 Uhr / Editiert am 9. November 2019, 17:42 Uhr / DIE ZEIT
Nr. 46/2019, 7. November 2019 / [9 Kommentare](#)



DEEP TROUBLE FOR DEEP LEARNING

BY DOUGLAS HEAVEN

Nature 574, 163-166 (2019)

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Researchers Find Flaws in High-Profile Study on Trees and Climate

Four independent groups say the work overestimates the carbon-absorbing benefits of global forest restoration, but the authors insist their original estimates are accurate.

Oct 17, 2019

KATARINA ZIMMER

www.the-scientist.com

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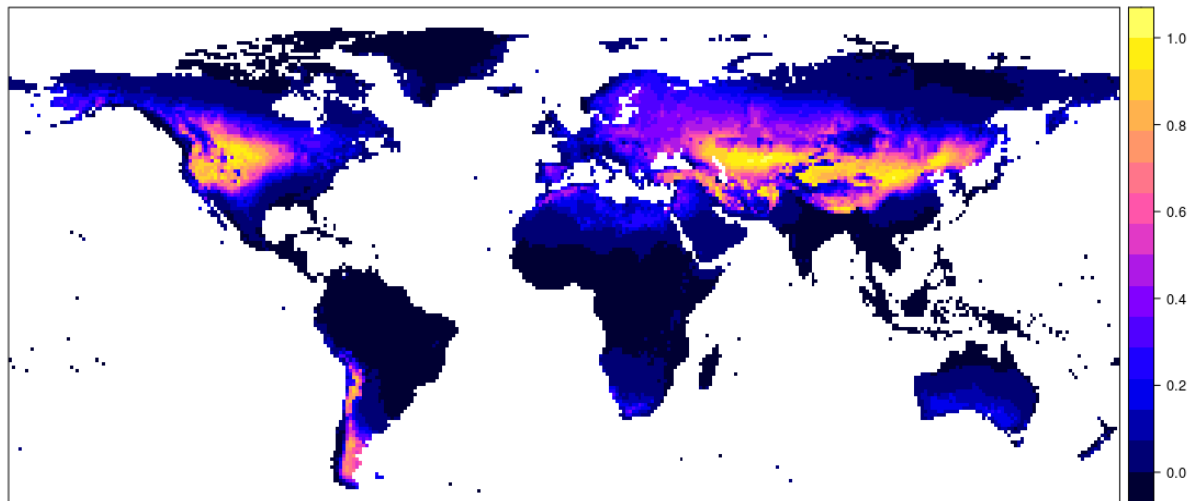
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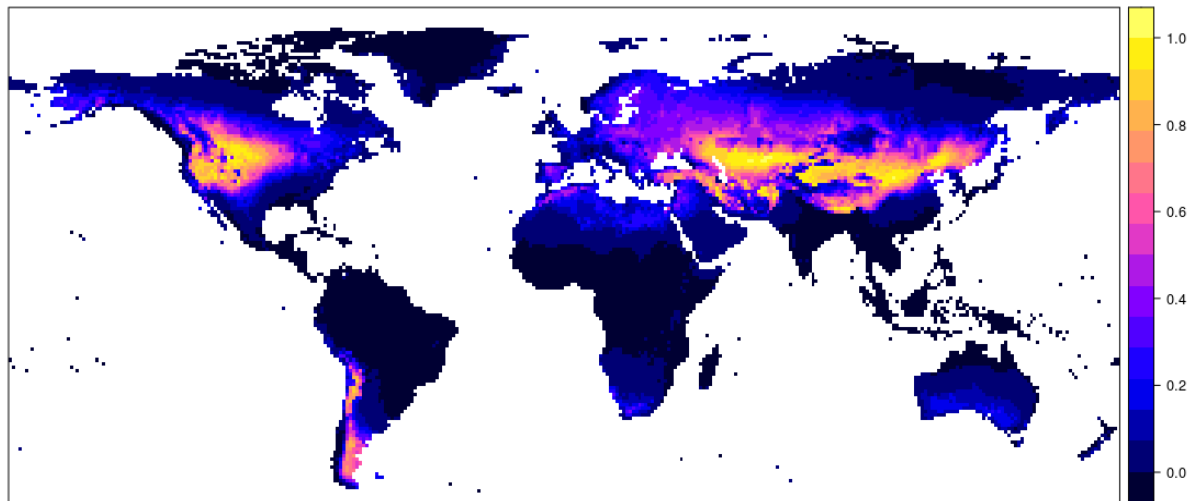
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Have we been too ambitious? Why might the models fail?

Largest challenge: predictions far beyond training samples



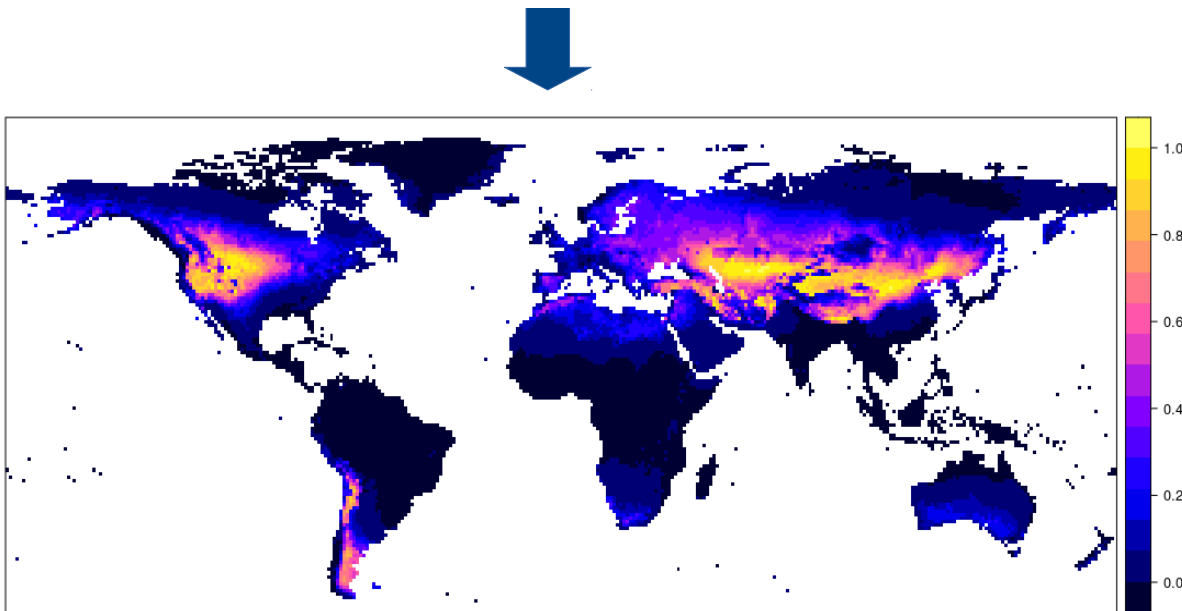
Largest challenge: predictions far beyond training samples



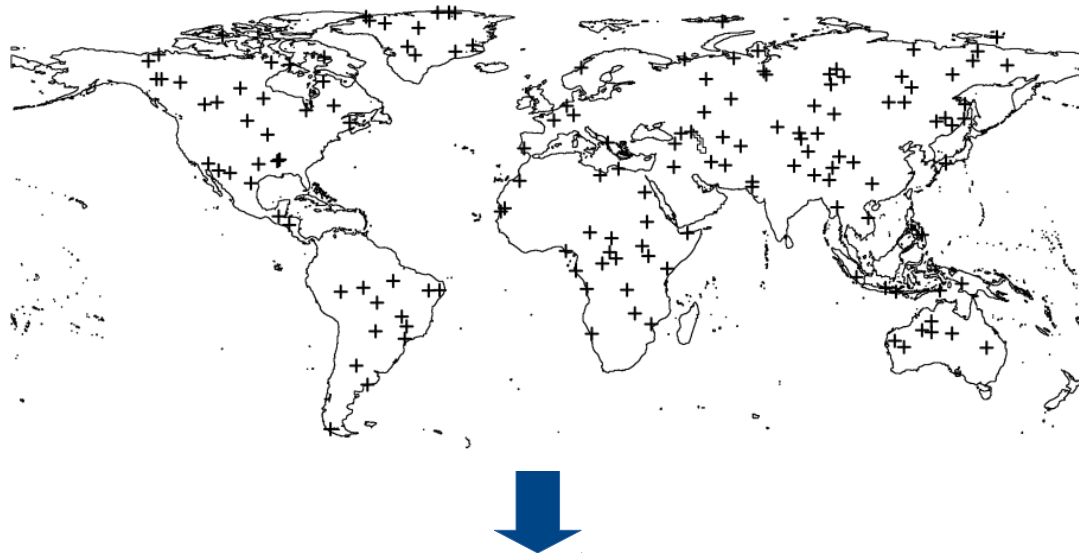
Largest challenge: predictions far beyond training samples



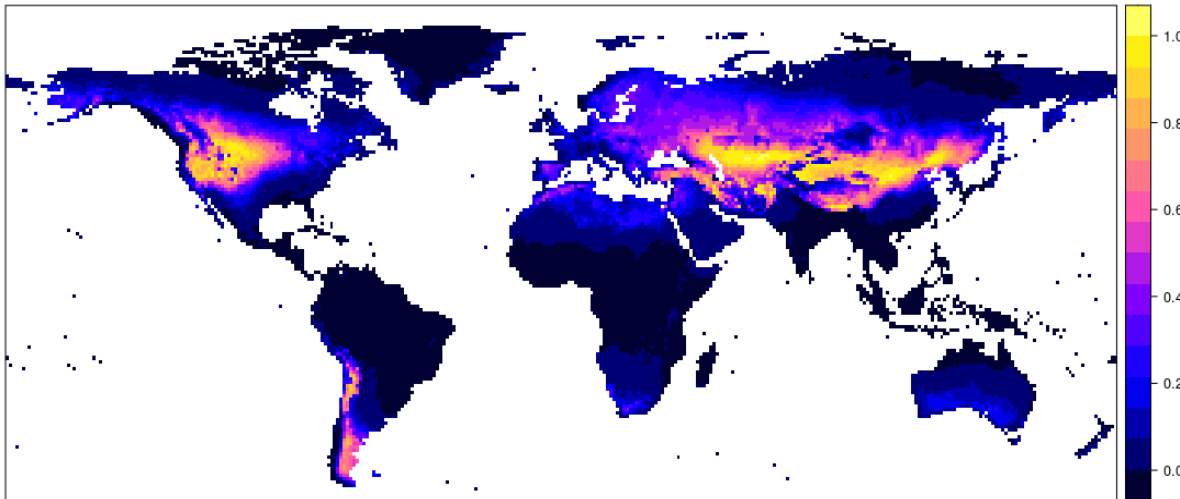
- Transfer to new space required



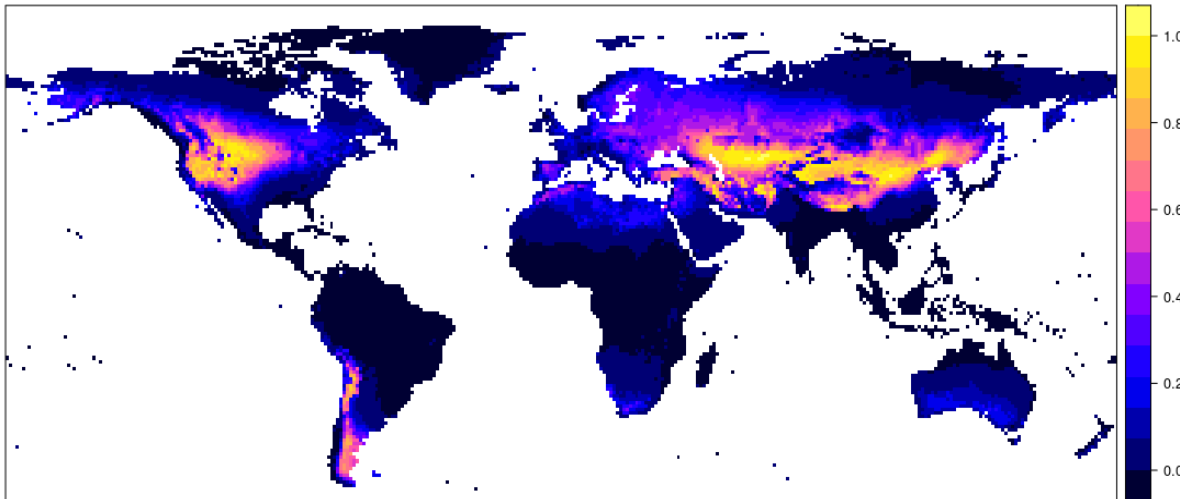
Largest challenge: predictions far beyond training samples



- Transfer to new space required
- New space might differ in environmental properties

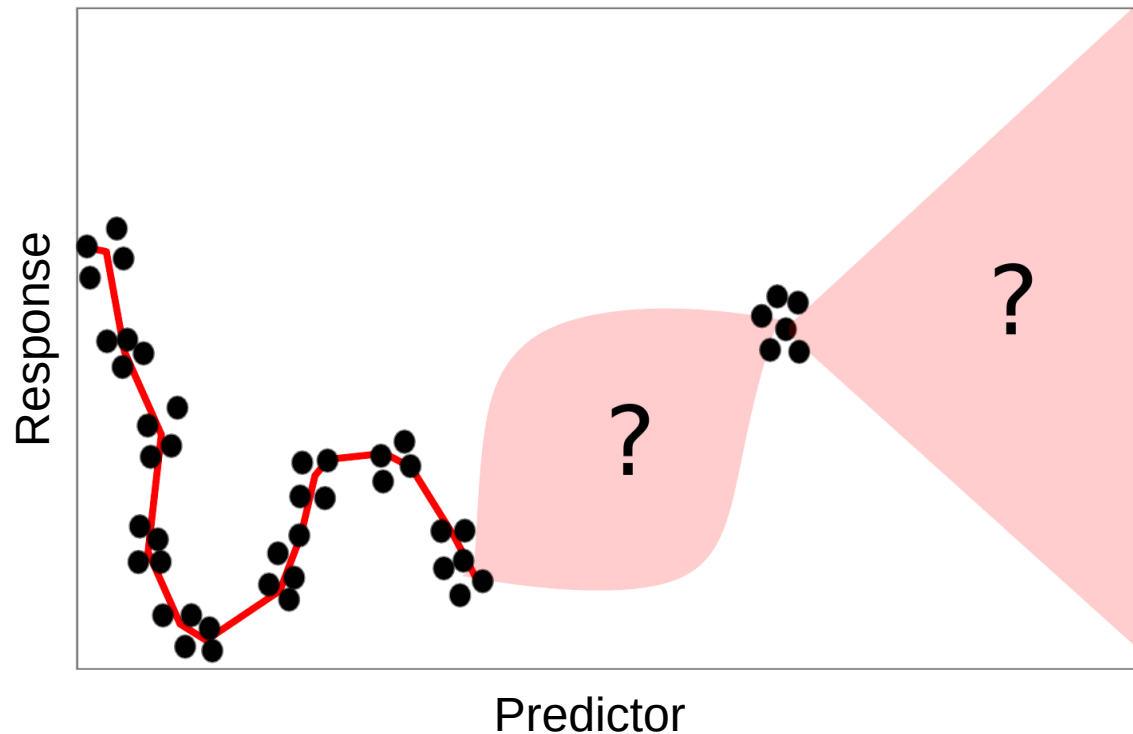


Largest challenge: predictions far beyond training samples



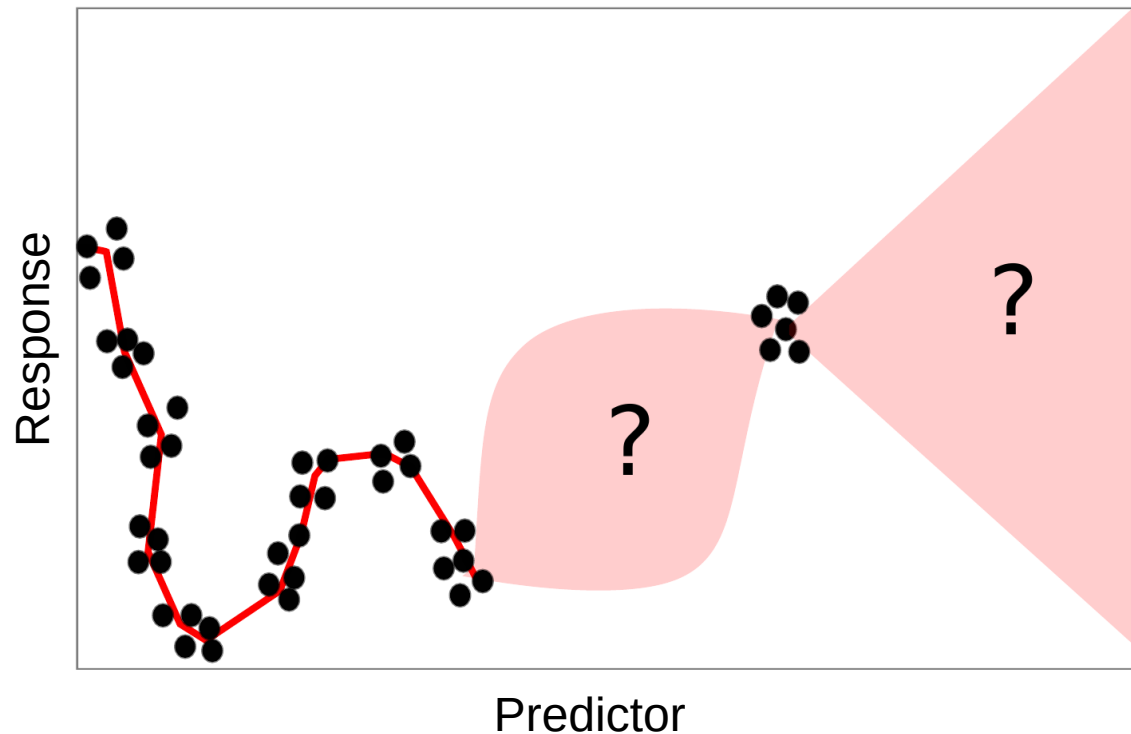
- Transfer to new space required
- New space might differ in environmental properties
- But what if the algorithm has never seen such properties?

Machine learning models are weak in extrapolations



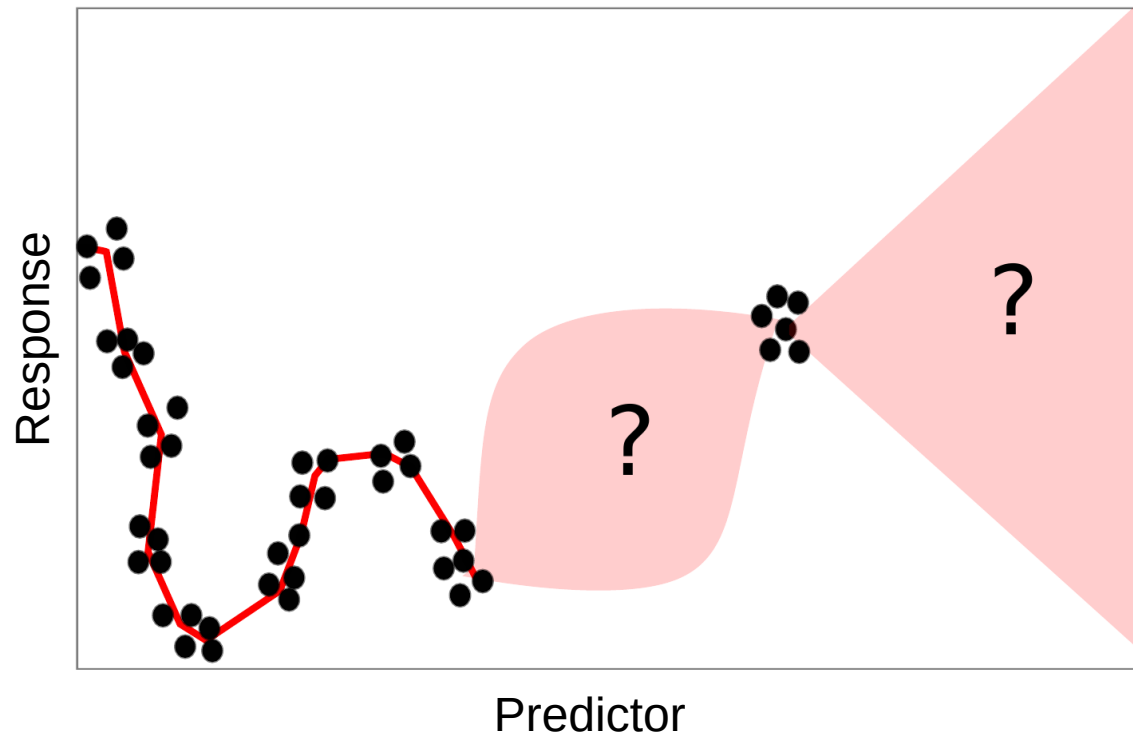
- Machine learning can fit very complex relationships.

Machine learning models are weak in extrapolations



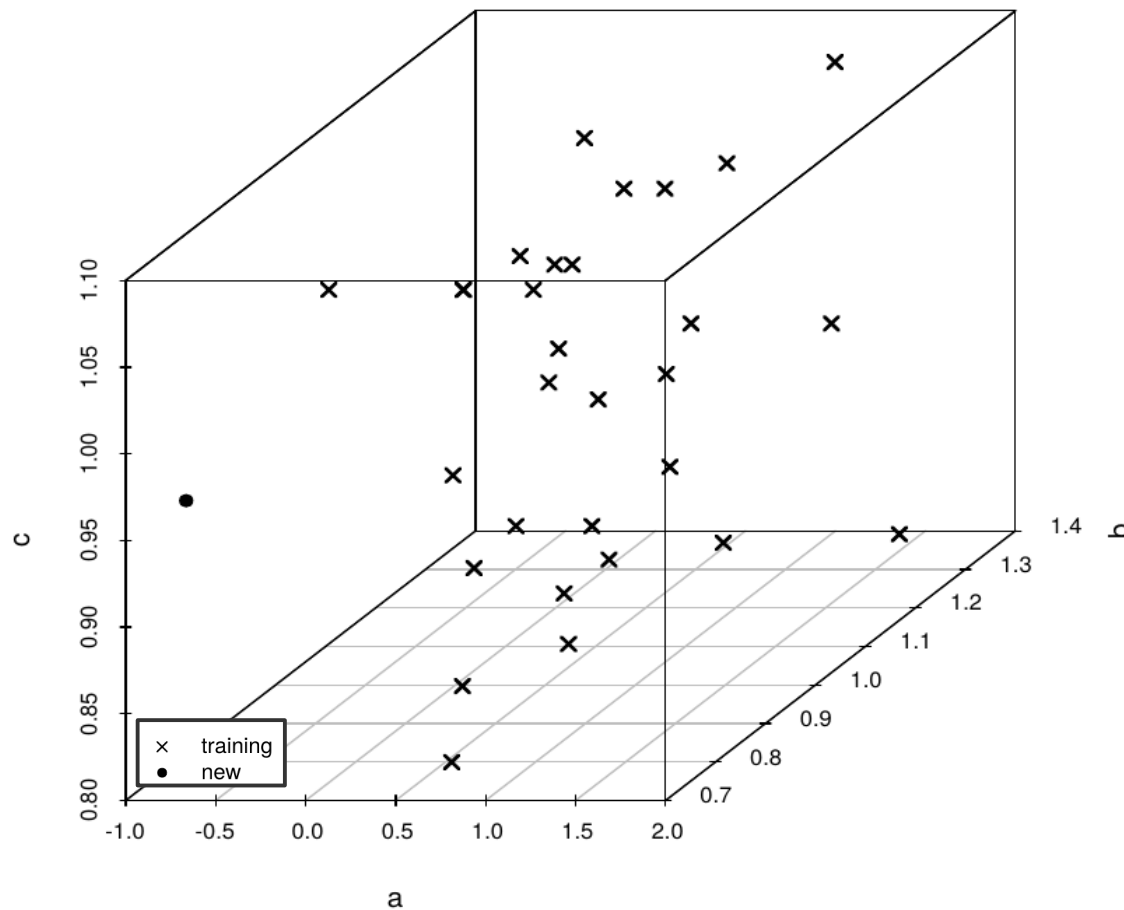
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- But gaps in predictor space are problematic (the model has no knowledge about these areas!)

Machine learning models are weak in extrapolations



- Machine learning can fit very complex relationships.
- But gaps in predictor space are problematic (the model has no knowledge about these areas!)
- A measure for “unknown space” is needed

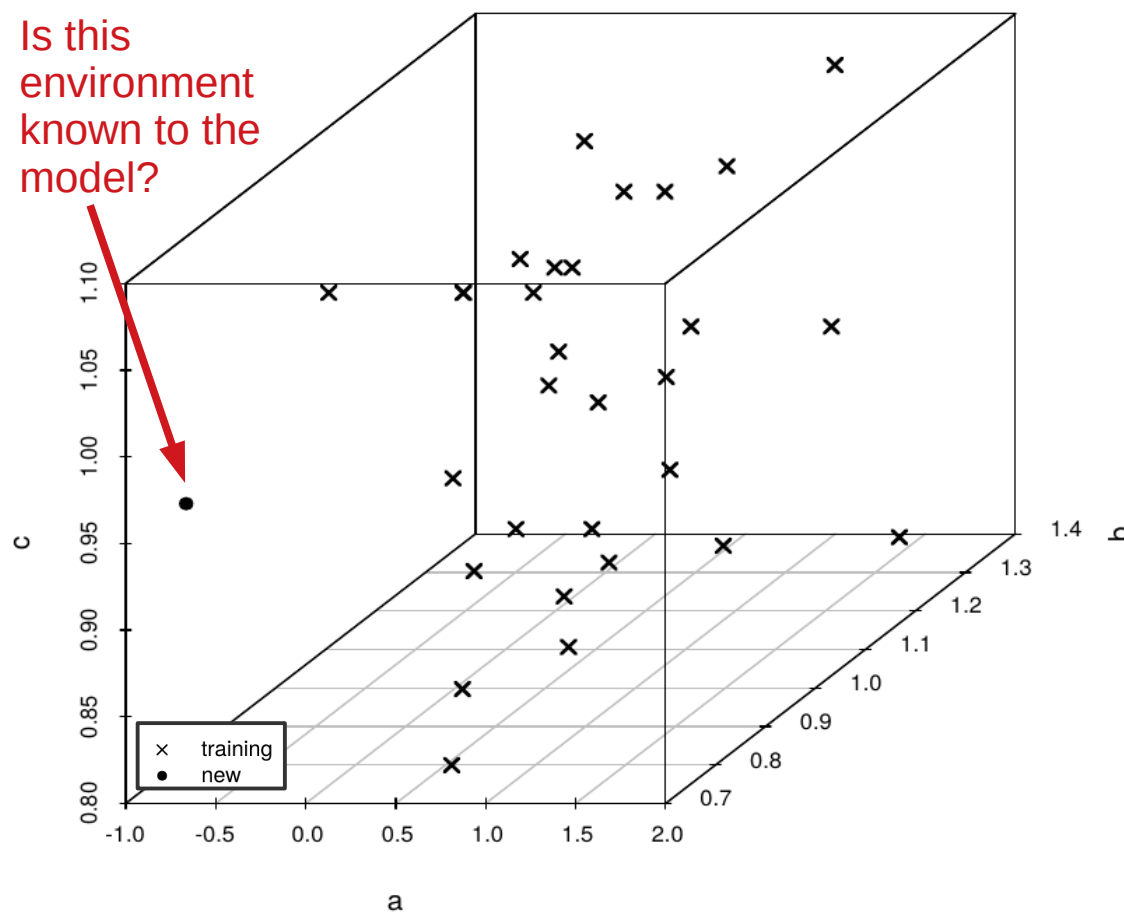
Distances in feature space as a measure for “unknown space”



- Unknown space: Environmental conditions that are very different from the training locations

*More details: <https://arxiv.org/abs/2005.07939>

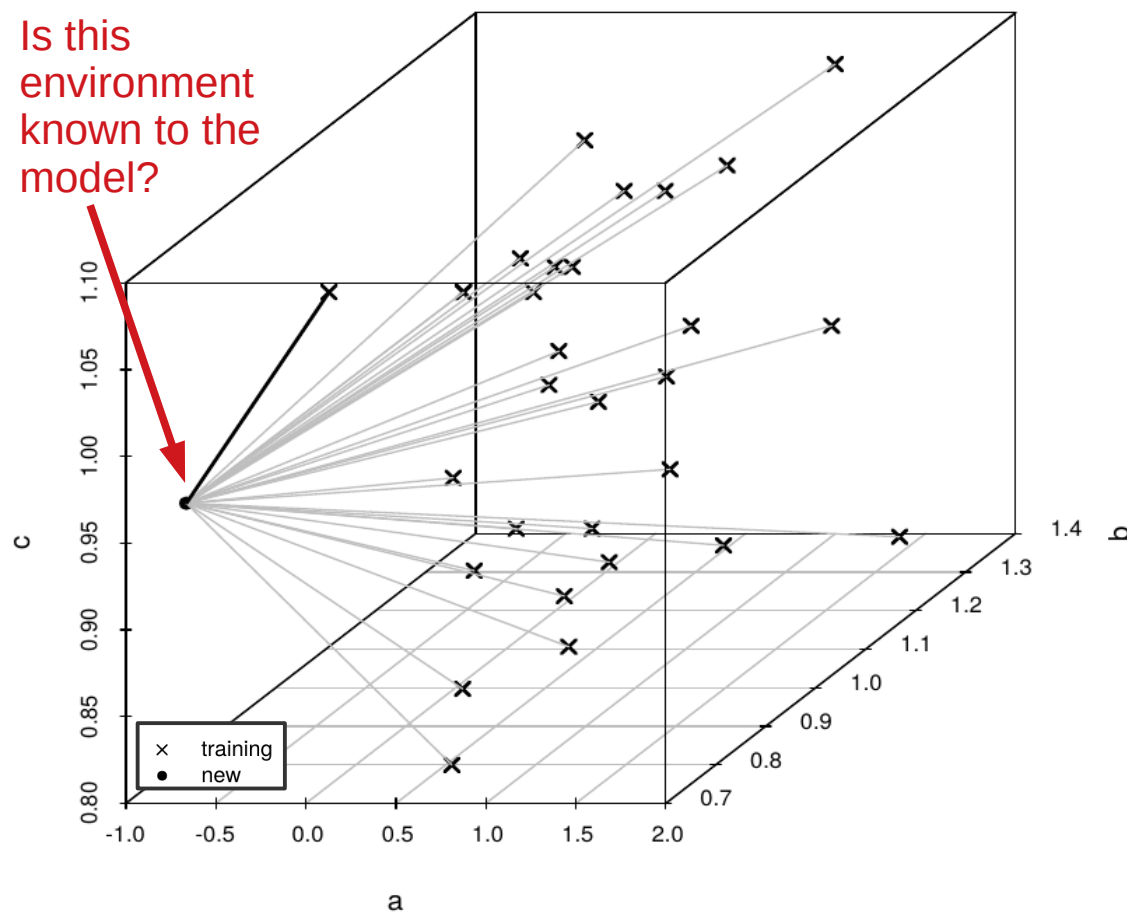
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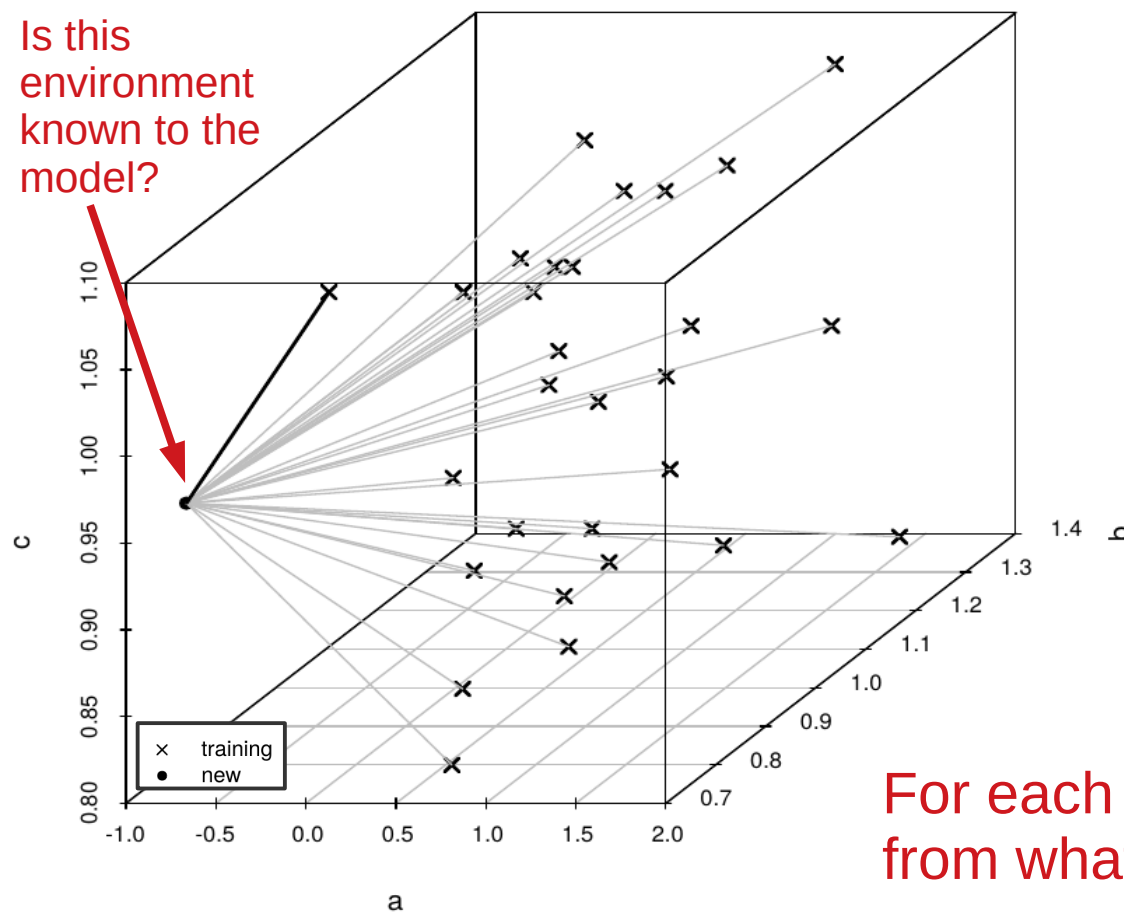
Distances in feature space as a measure for “unknown space”



- Unknown space: Environmental conditions that are very different from the training locations
- Suggestion: Dissimilarity Index based on distances in the (weighted) predictor space*

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Distances in feature space as a measure for “unknown space”



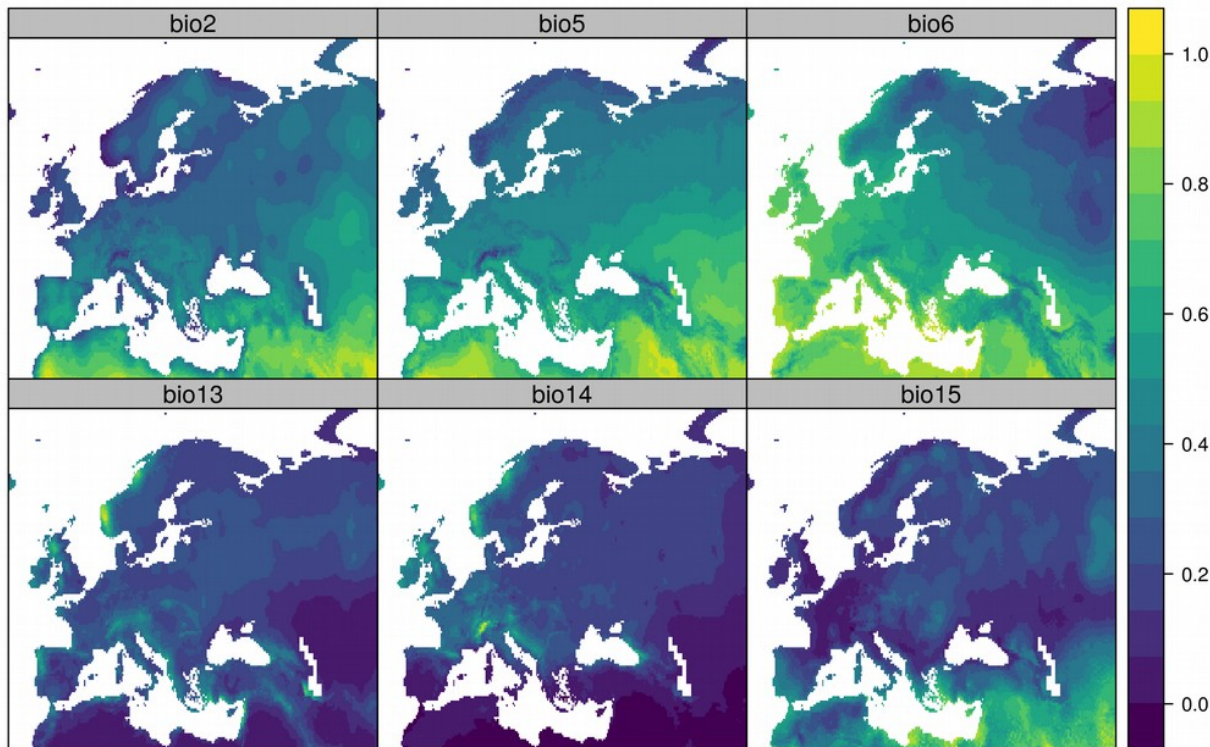
- Unknown space: Environmental conditions that are very different from the training locations
- Suggestion: Dissimilarity Index based on distances in the (weighted) predictor space*

For each new location/pixel: how distant is it from what the algorithm has seen?

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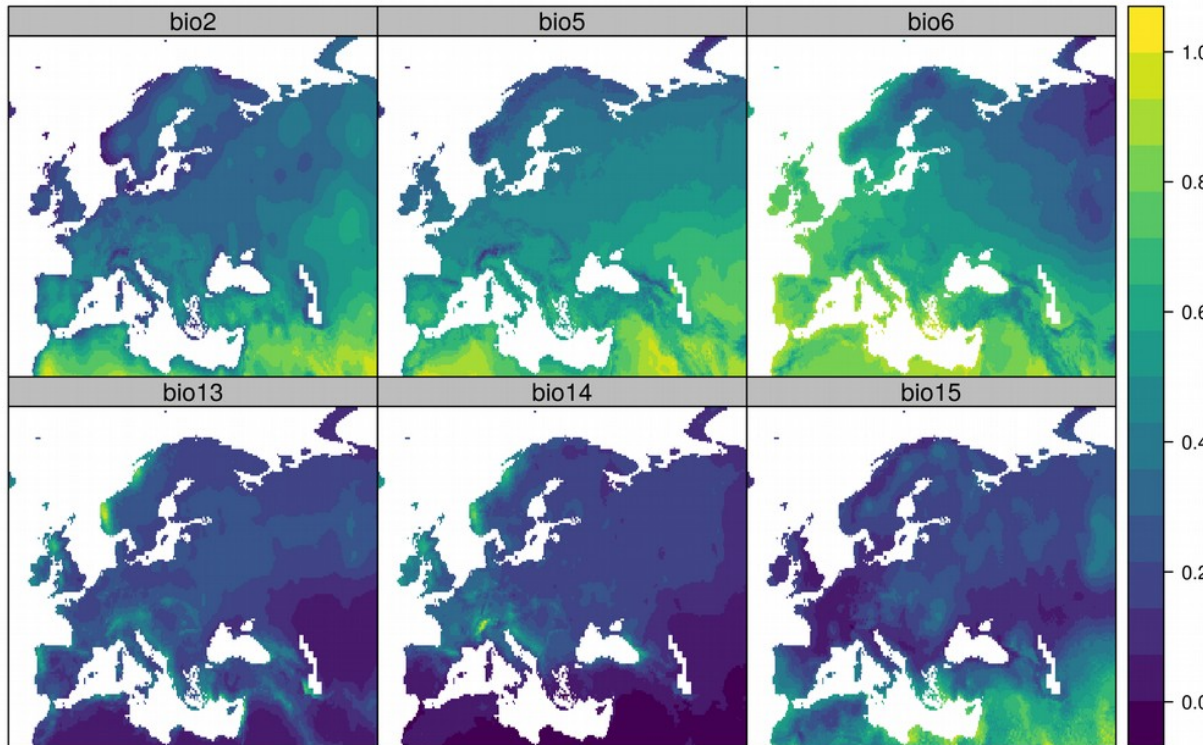
Mapping the area of applicability - Example

Predictors

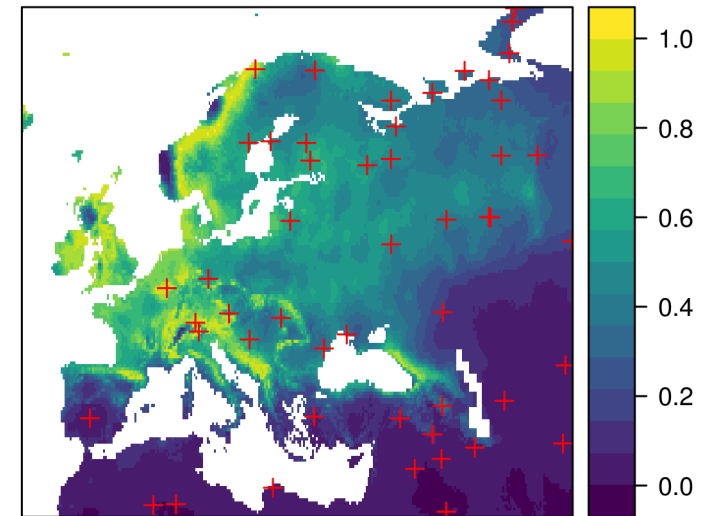


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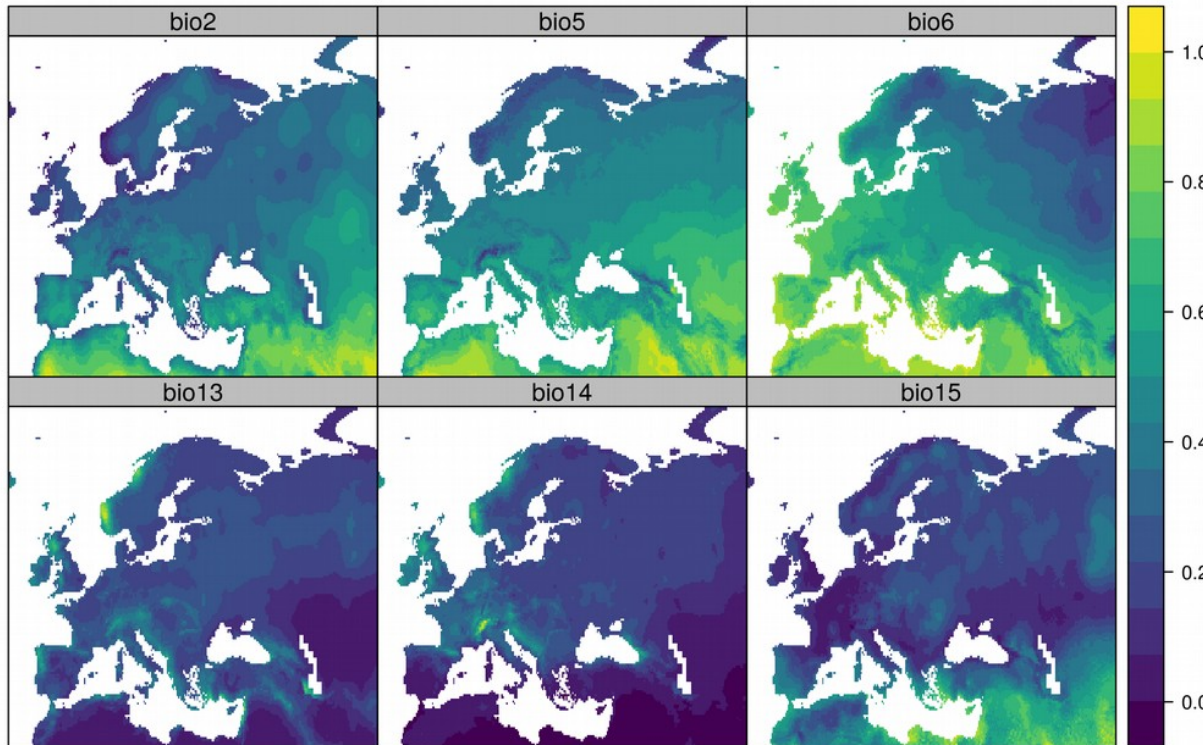


Virtual Response and simulated samples

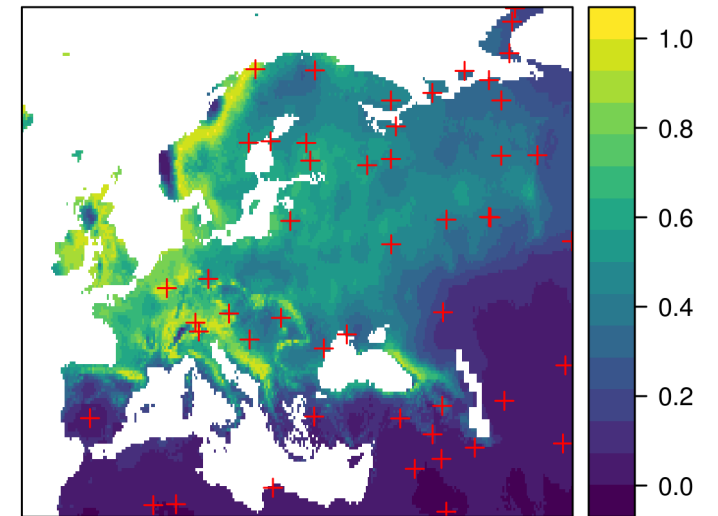


Mapping the area of applicability - Example

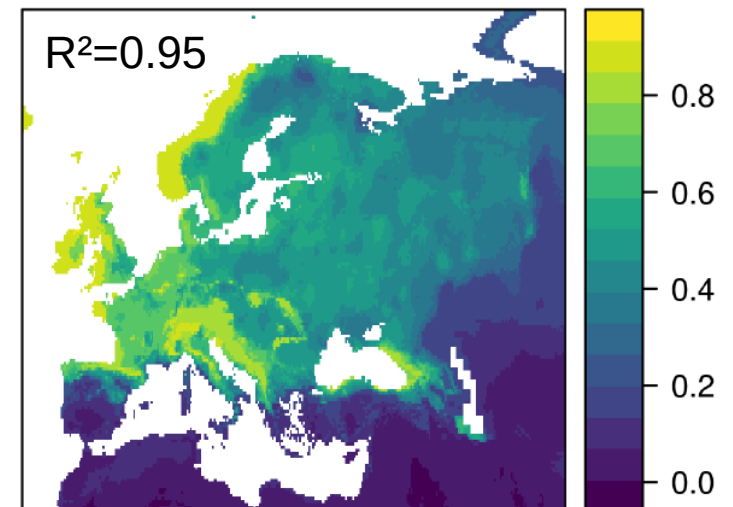
Predictors



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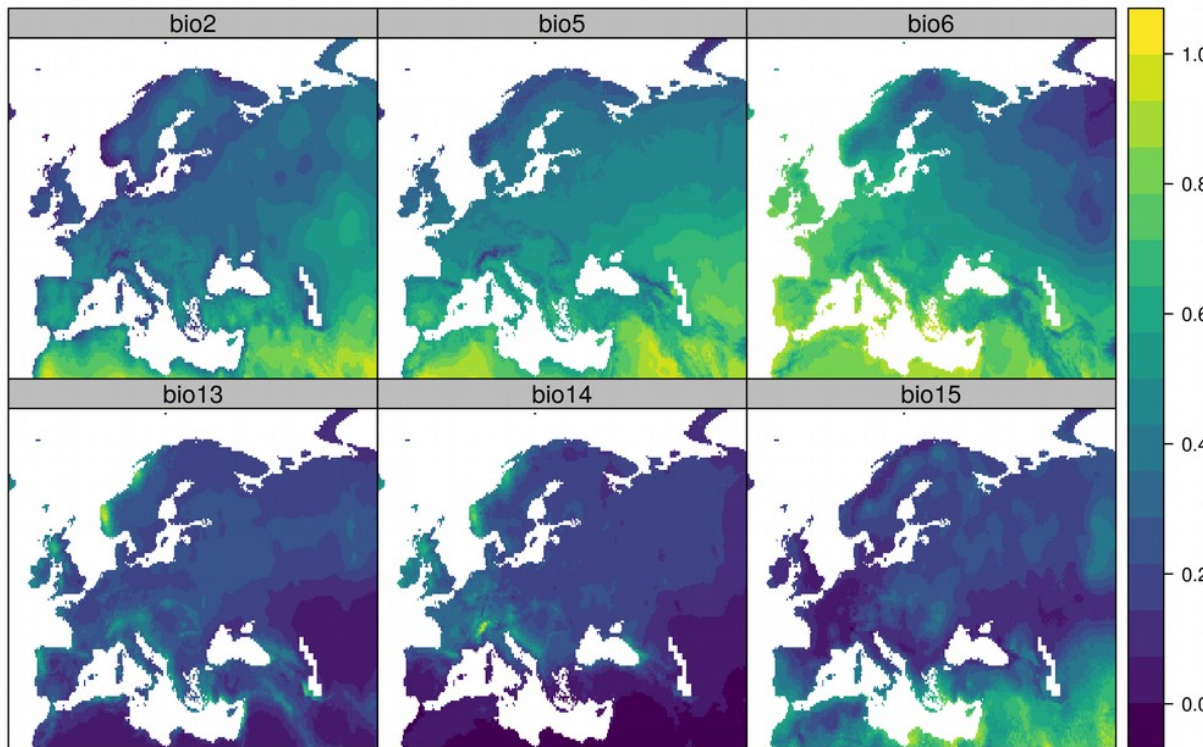


Prediction

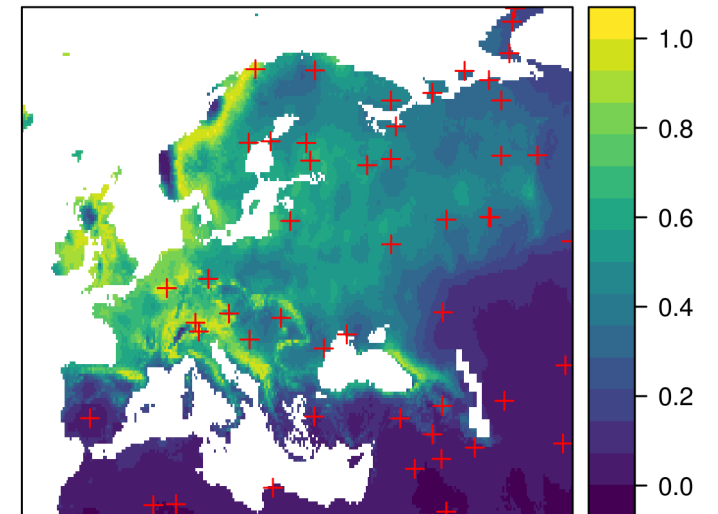


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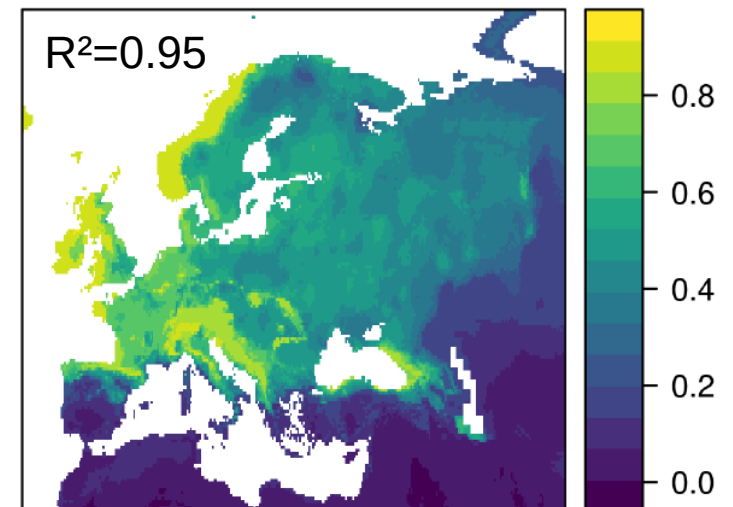
Predictors



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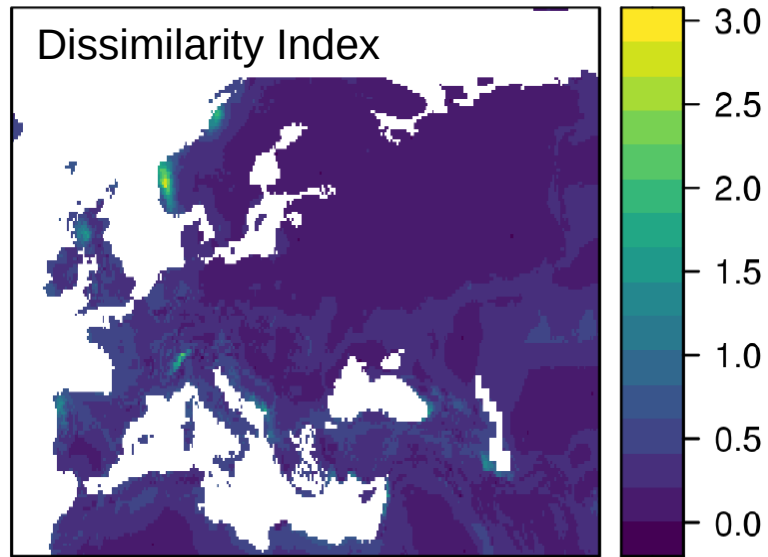


Prediction

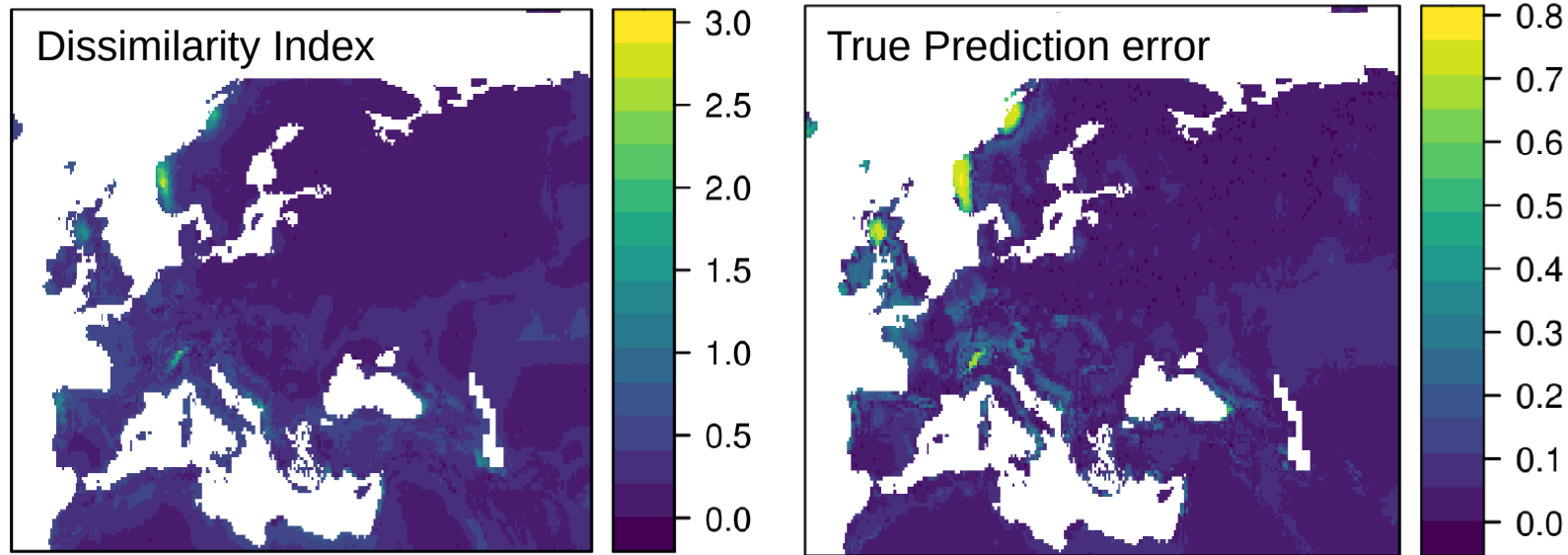


Where can we trust the predictions
and where should we better not?

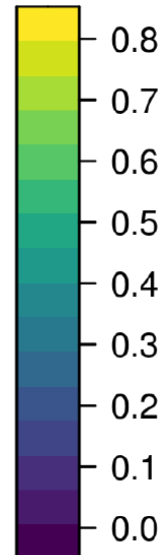
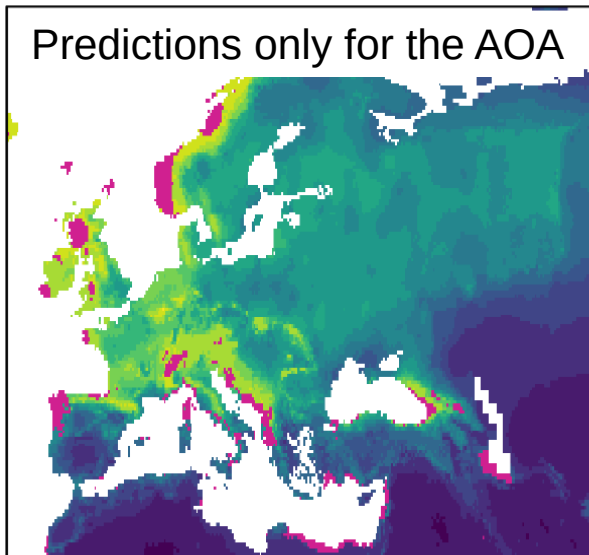
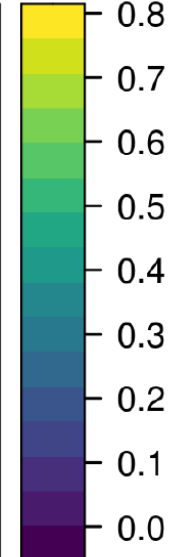
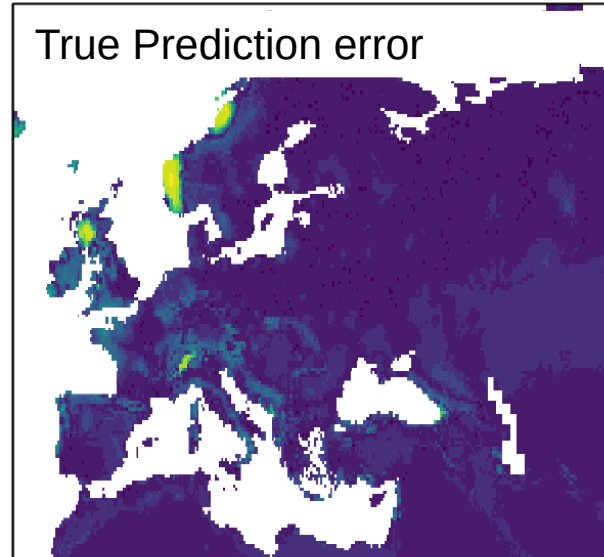
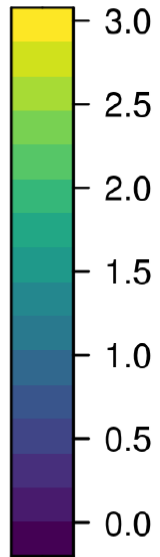
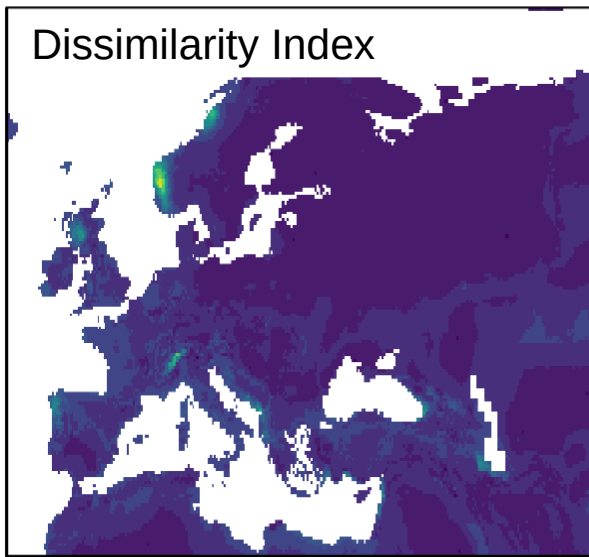
Mapping the area of applicability - Example



Mapping the area of applicability - Example



Mapping the area of applicability - Example



Threshold = DI of cross-validated training data

DI < threshold = inside AOA

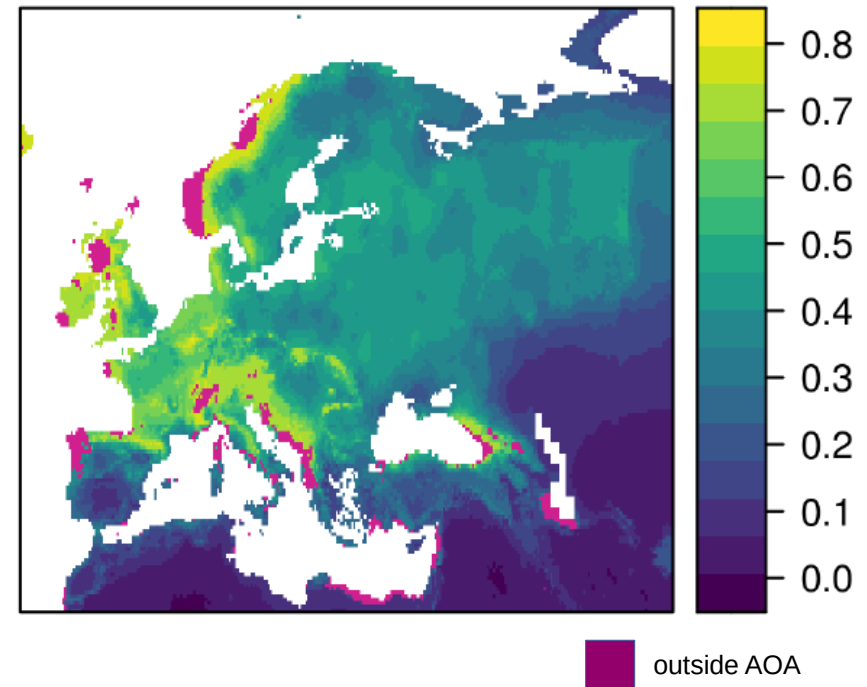
DI > threshold = outside AOA

Outside AOA

Why is it relevant to map the area of applicability?

Results are not just nice maps but used for...

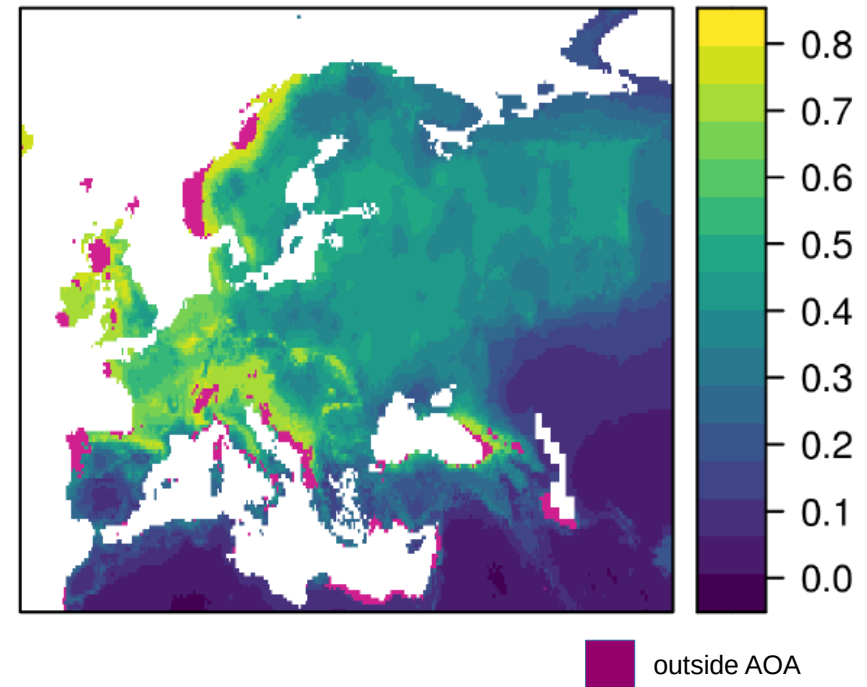
- subsequent modeling
- nature conservation
- risk assessment
- ...



Why is it relevant to map the area of applicability?

Results are not just nice maps but used for...

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Predictions should only be presented for the area of applicability to avoid error propagation or misplanning (and to keep trust in the methods)!

More information

- Meyer H, Pebesma E: Predicting into unknown space? Estimating the area of applicability of spatial prediction models.
<https://arxiv.org/abs/2005.07939>
- Method implemented in the R Package “CAST”:
<https://CRAN.R-project.org/package=CAST>
- Tutorial: https://github.com/HannaMeyer/OpenGeoHub_2020