Interpretable ML for biodiversity

An introduction using species distribution models

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MAIN GOALS

1. How do we produce a model?
2. How do we convey that it works?
3. How do we talk about how it makes predictions?
4. How do we use it to guide actions?

THE STEPS

1. Get data about species occurrences
2. Build a classifier and make it as good as we can
3. Measure its performance
4. Explain some predictions
5. Generate counterfactual explanations
6. Briefly discuss ensemble models

BUT WHY...

... think of SDM as a ML problem? Because they are! We want to learn a predictive algorithm from data

... the focus on explainability? We cannot ask people to *trust* - we must *convince* and *explain*

§ 1

Problem statement

THE PROBLEM IN ECOLOGICAL TERMS

We have information about a species

THE PROBLEM IN OTHER WORDS

We have a series of observations $y \in \mathbb{B}$, and predictors variables $\mathbf{X} \in \mathbb{R}$

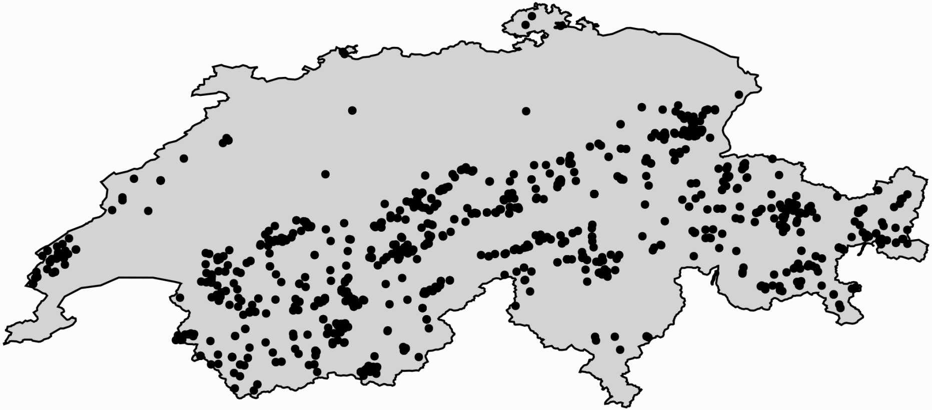
We want to find an algorithm $f(\mathbf{x}) = \hat{y}$ that results in the distance between $\hat{y}$ and y being *small*

SETTING UP THE DATA FOR OUR EXAMPLE

The predictor data will come from CHELSA2 - we will start with the 19 BioClim variables

We will use data on observations of *Turdus torquatus* in Switzerland, downloaded from the copy of the eBird dataset on GBIF

THE OBSERVATION DATA



PROBLEM!

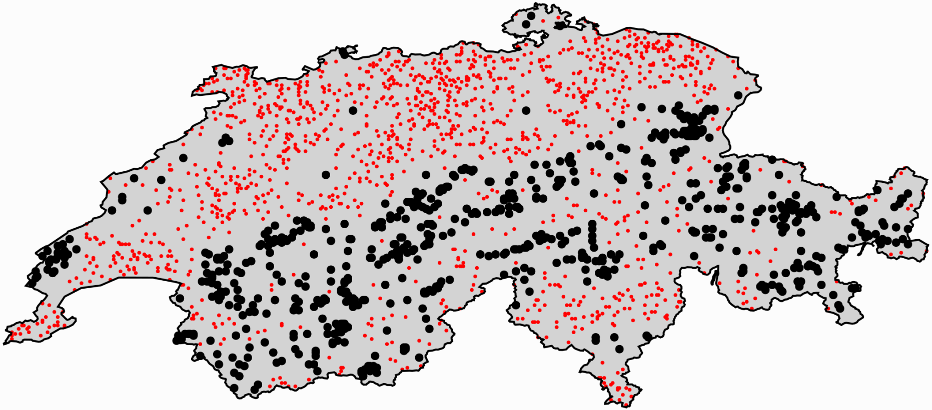
We want $\hat{y} \in \mathbb{B}$, and so far we are missing negative values

SOLUTION!

pseudo-absences

what are the assumptions we make

THE (INFLATED) OBSERVATION DATA



§ 2

Training the model

$$P(+|x) = \frac{P(+)}{P(x)} P(x|+)$$

$$\hat{y} = \operatorname{argmax}_j P(\mathbf{c}_j) \prod_i P(\mathbf{x}_i|\mathbf{c}_j)$$

$$P(x|+) = \operatorname{pdf}(x, \mathcal{N}(\mu_+, \sigma_+))$$

SETUP

Can we train the model

assumes parallel universes with slightly less data

is the model good?

NULL CLASSIFIERS

coin flip

no skill

constant

Model	MCC	PPV	NPV	DOR	Accuracy
noskill	0.0	0.338178	0.661822	1.0	0.552373
coinflip	-0.323643	0.338178	0.338178	0.261102	0.338178
constantpositive	0.0	0.338178	NaN	NaN	0.338178
constantnegative	0.0	NaN	0.661822	NaN	0.661822

CROSS-VALIDATION STRATEGY

k-fold

validation / training / testing

CROSS-VALIDATION RESULTS

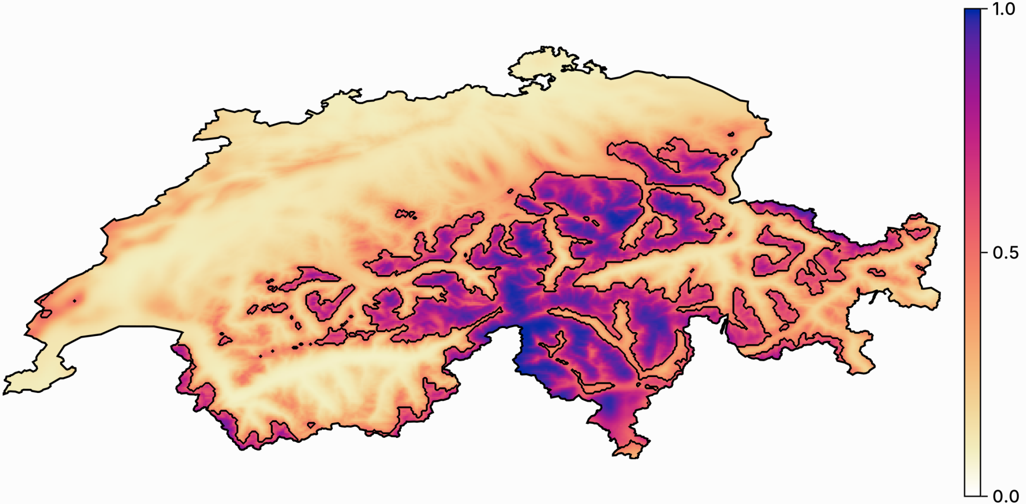
Model	MCC	PPV	NPV	DOR	Accuracy
noskill	0.0	0.338178	0.661822	1.0	0.552373
coinflip	-0.323643	0.338178	0.338178	0.261102	0.338178
constantpositive	0.0	0.338178	NaN	NaN	0.338178
constantnegative	0.0	NaN	0.661822	NaN	0.661822
Validation	0.285042	0.573912	0.739042	3.97394	0.698661
Training	0.287722	0.57633	0.73963	3.869	0.699451

WHAT TO DO IF THE MODEL IS TRAINABLE?

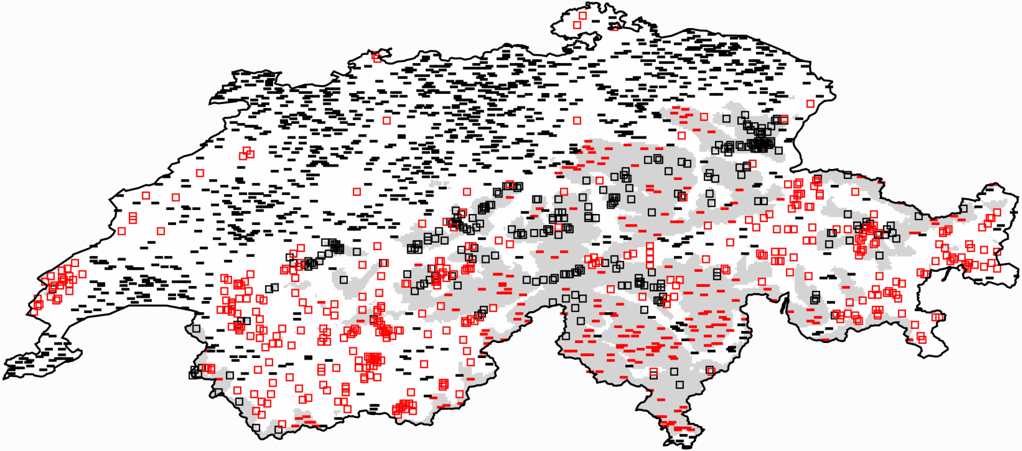
train it!

re-use the full dataset

INITIAL PREDICTION



HOW IS THIS MODEL WRONG?



CAN WE IMPROVE ON THIS MODEL?

variable selection

data transformation

hyper-parameters tuning

will focus on the later (same process for the two above)

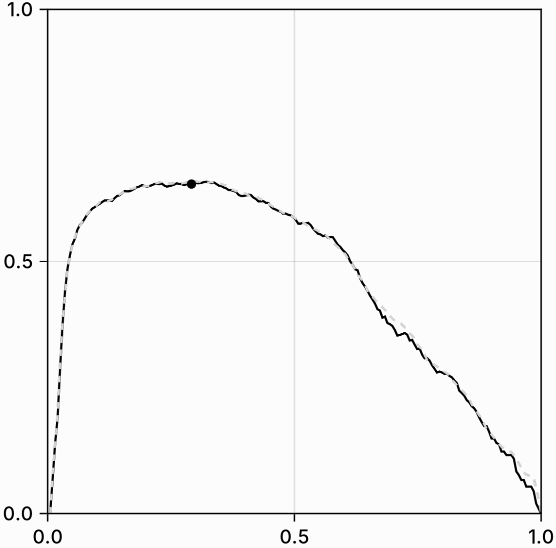
MOVING THESHOLD CLASSIFICATION

p plus > p minus means threshold is 0.5

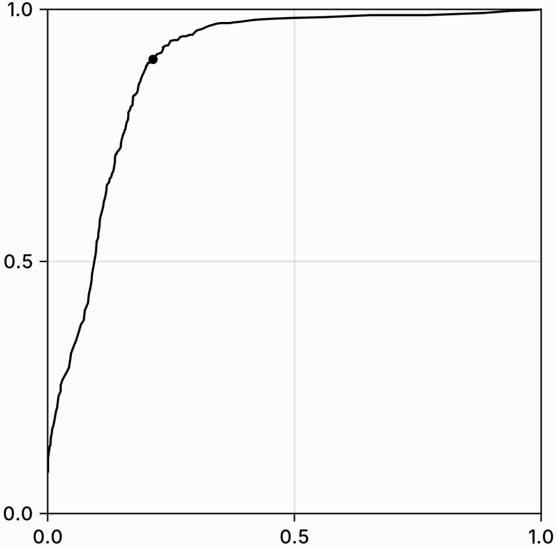
is it?

how do we check this

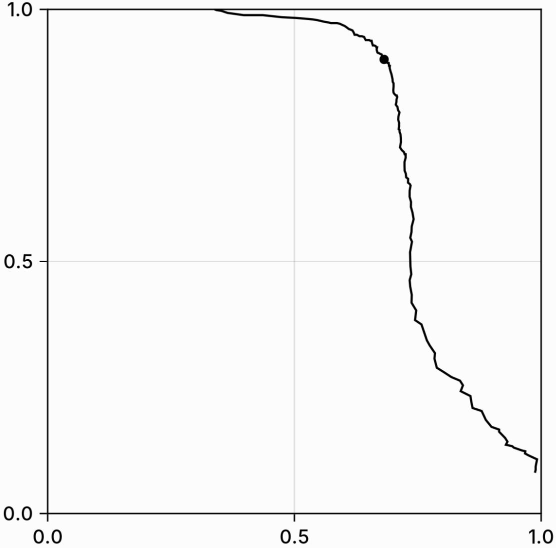
LEARNING CURVE FOR THE THRESHOLD



RECEIVER OPERATING CHARACTERISTIC



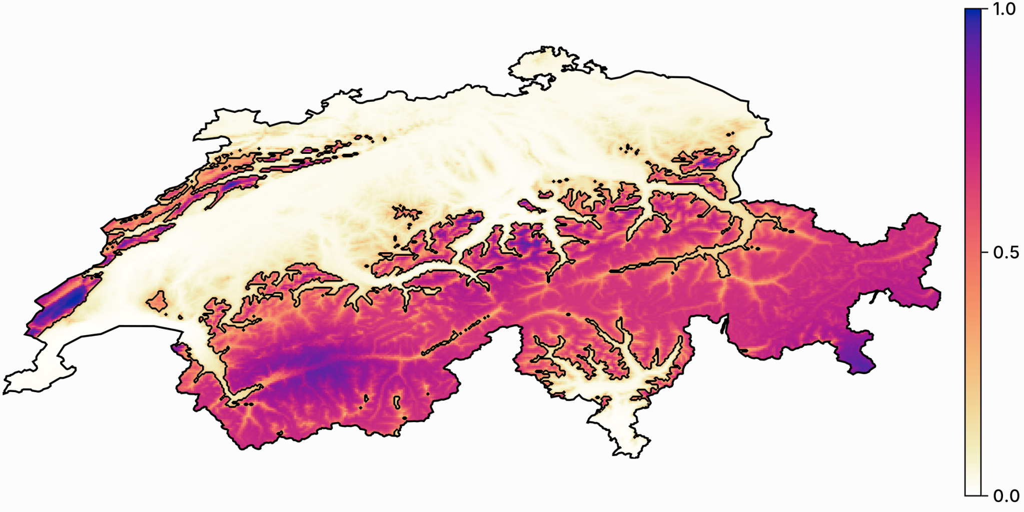
PRECISION-RECALL CURVE



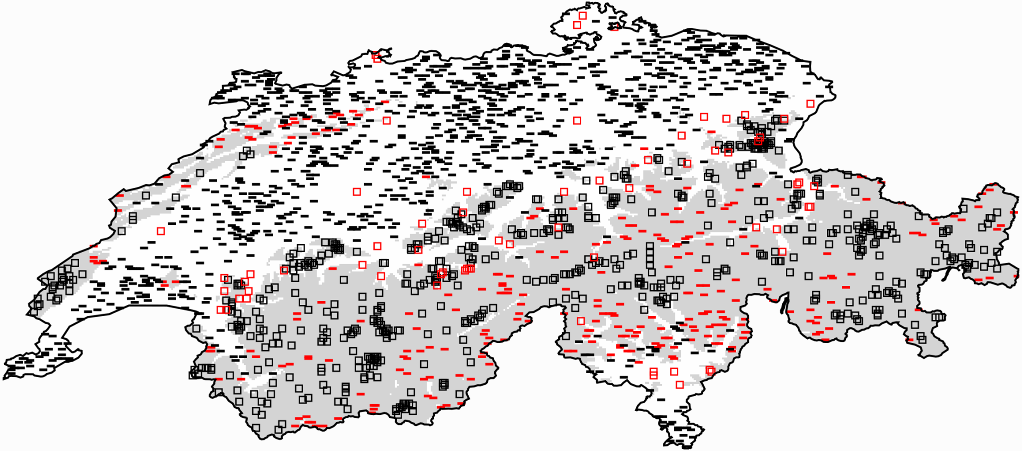
REVISITING THE MODEL PERFORMANCE

Model	MCC	PPV	NPV	DOR	Accuracy
noskill	0.0	0.338178	0.661822	1.0	0.552373
coinflip	-0.323643	0.338178	0.338178	0.261102	0.338178
constantpositive	0.0	0.338178	NaN	NaN	0.338178
constantnegative	0.0	NaN	0.661822	NaN	0.661822
Previous	0.285042	0.573912	0.739042	3.97394	0.698661
Validation	0.65469	0.682064	0.940772	38.1561	0.825594
Training	0.658932	0.686247	0.941019	34.9715	0.827627

UPDATED PREDICTION



HOW IS THIS MODEL BETTER?



REVISITING ASSUMPTIONS

- pseudo-absences
- not just a statistical exercise

VARIABLE IMPORTANCE

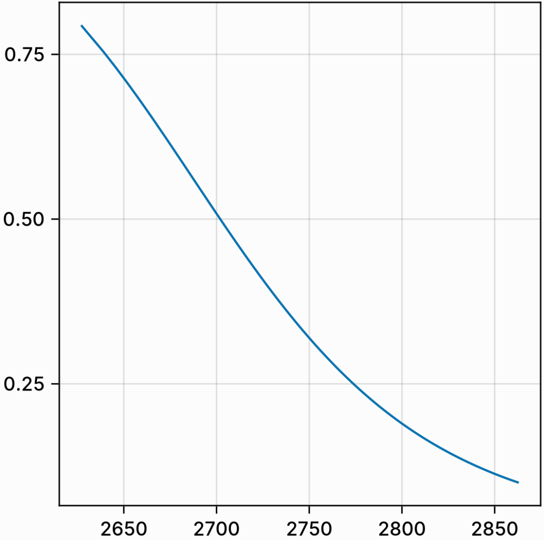
BIO	Import.
11.0	0.342392
5.0	0.292015
10.0	0.254812
1.0	0.110781

§ 3

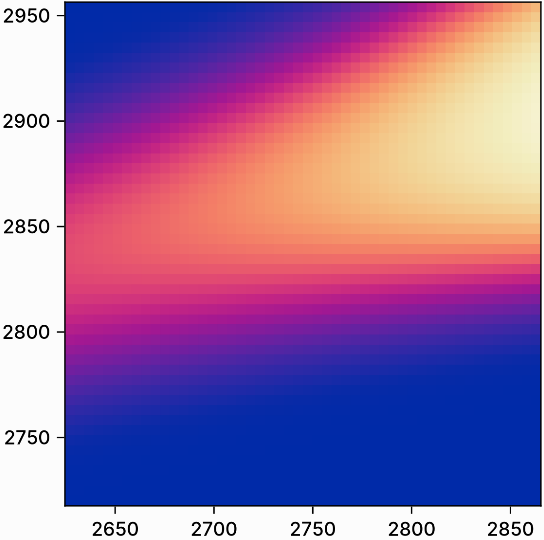
But why?

AN ECOLOGY TOOL: PARTIAL RESPONSE CURVES

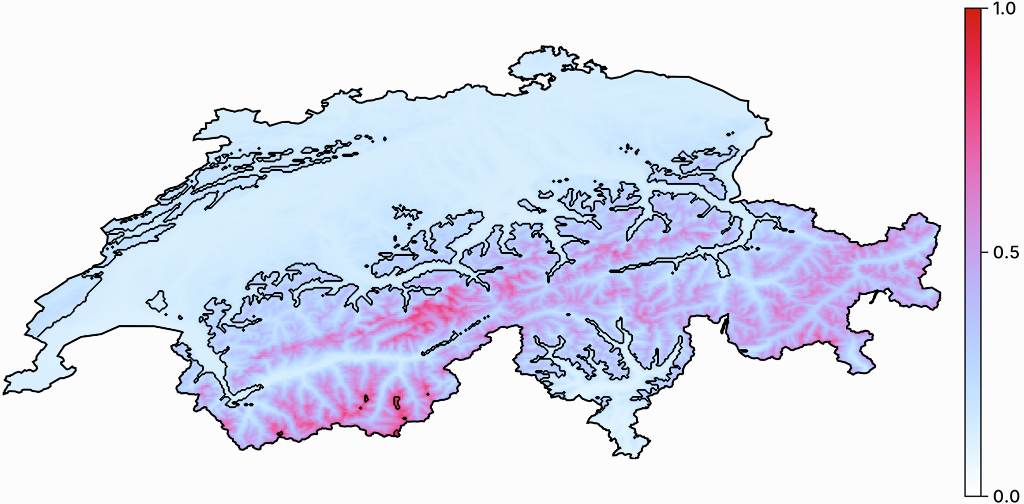
EXAMPLE WITH TEMPERATURE



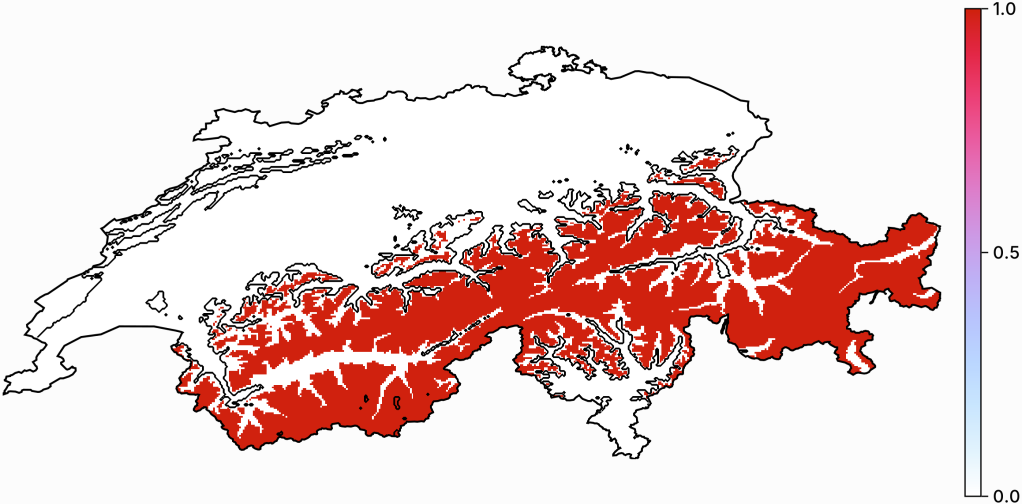
EXAMPLE WITH TWO VARIABLES



SPATIALIZED PARTIAL RESPONSE PLOT



SPATIALIZED PARTIAL RESPONSE (BINARY OUTCOME)



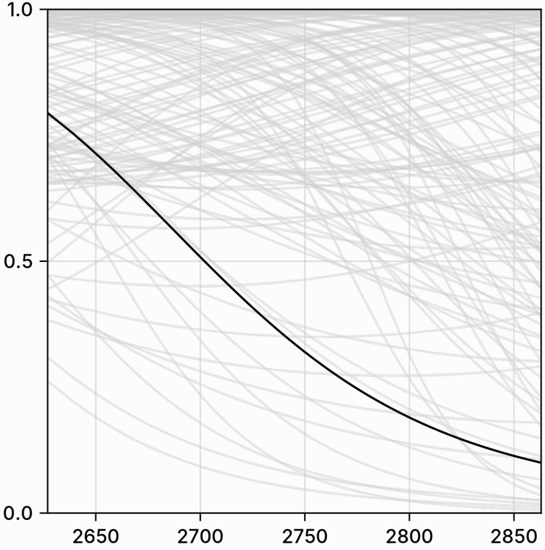
Averaging the variables is masking a lot of variability!

Alternative solution:

1. Generate a grid for all the variables
2. For all combinations in this grid, use it as the stand-in for the variables to replace

In practice: Monte-Carlo on a reasonable number of samples.

EXAMPLE

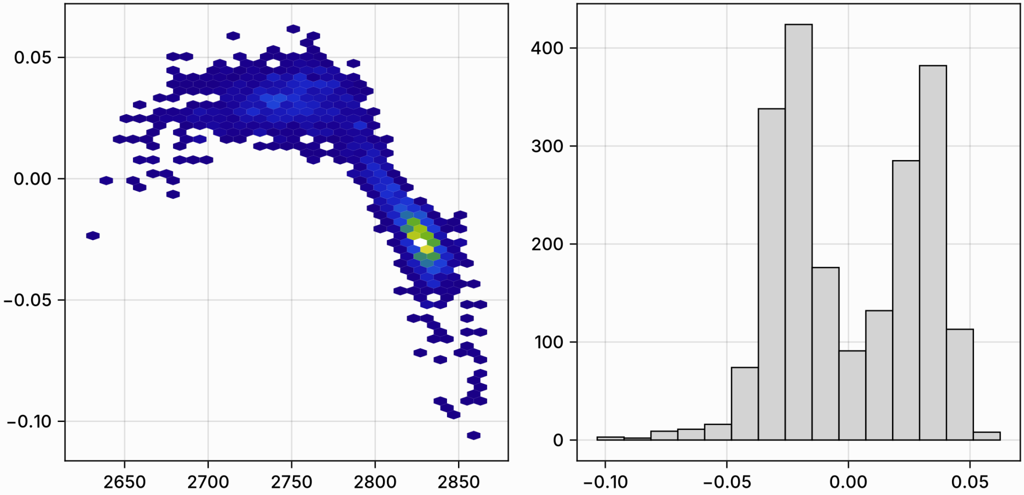


LIMITATIONS

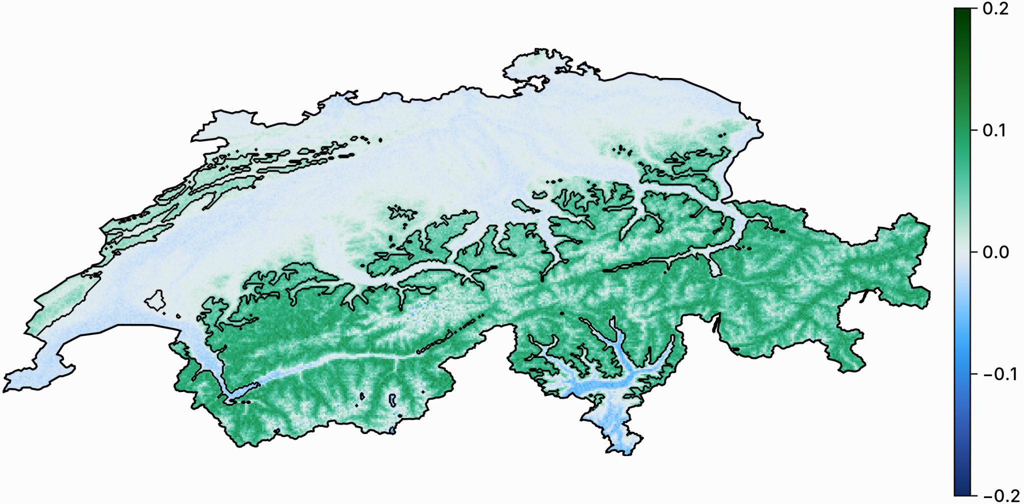
- partial responses can only generate model-level information
- they break the structure of values for all predictors at the scale of a single observation
- their interpretation is unclear

EXAMPLE

RESPONSE CURVES REVISITED

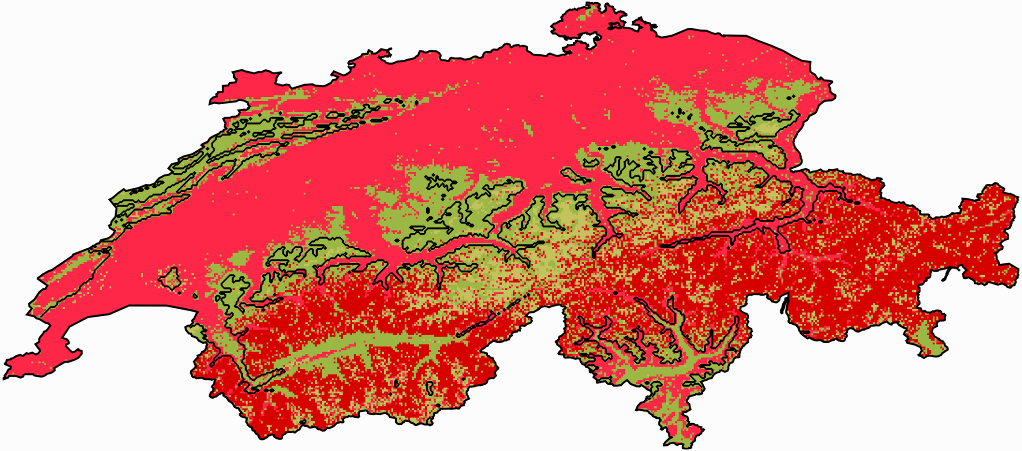


ON A MAP



BIO	Import.	Shap. imp.
5.0	0.292015	0.358287
11.0	0.342392	0.317696
1.0	0.110781	0.163154
10.0	0.254812	0.160862

MOST IMPORTANT PREDICTOR



§ 4

What if?

what they are

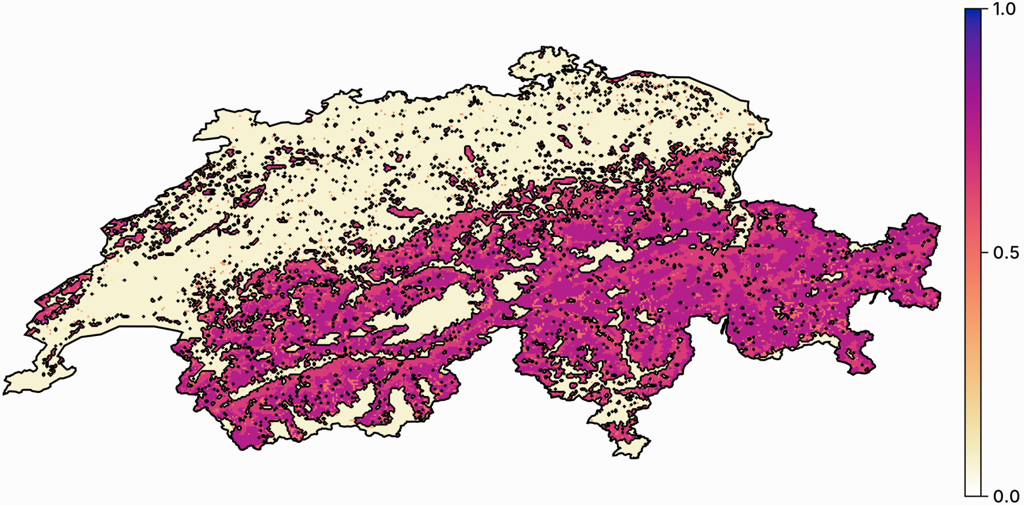
SETTING UP A NEW PROBLEM

- land use
- decision tree - very easy to overfit
- at most 18 nodes of depth at most 7
- same process

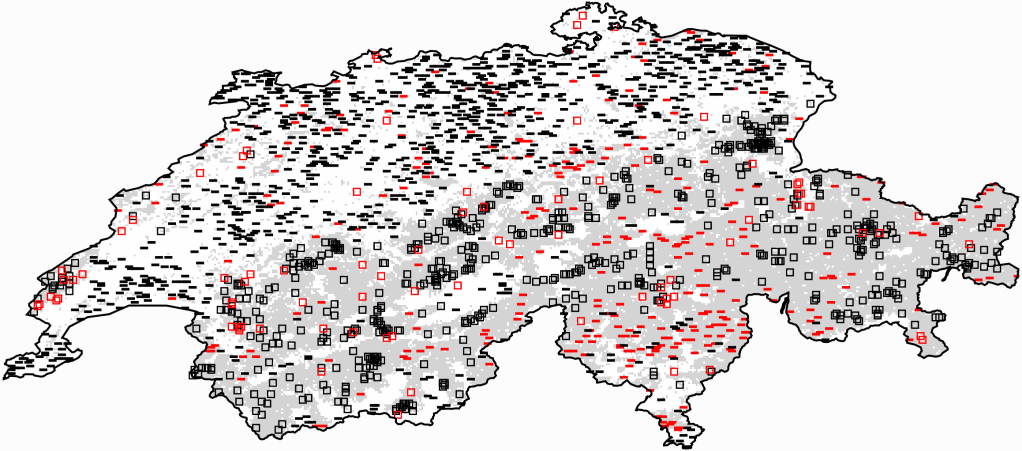
VARIABLE IMPORTANCE

Variable	Relative importance
Evergreen/Deciduous Needleleaf Trees	0.580133
Herbaceous Vegetation	0.377976
Urban/Built-up	0.0251986
Snow/Ice	0.0166925
Evergreen Broadleaf Trees	0.0

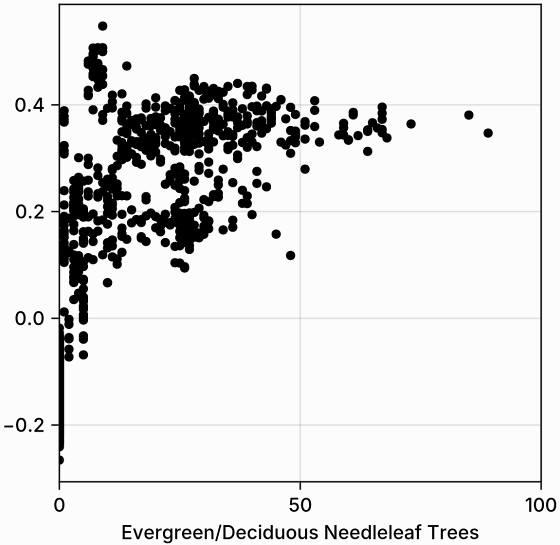
VISUALIZING THE PREDICTION



VISUALIZING THE ERRORS



PARTIAL RESPONSE (SHAPLEY)



GENERATING A COUNTERFACTUAL

EVALUATING THE COUNTERFACTUALS

THE RASHOMON EFFECT

- different but equally likely alternatives
- happens at all steps in the process

§ 5

Ensemble models

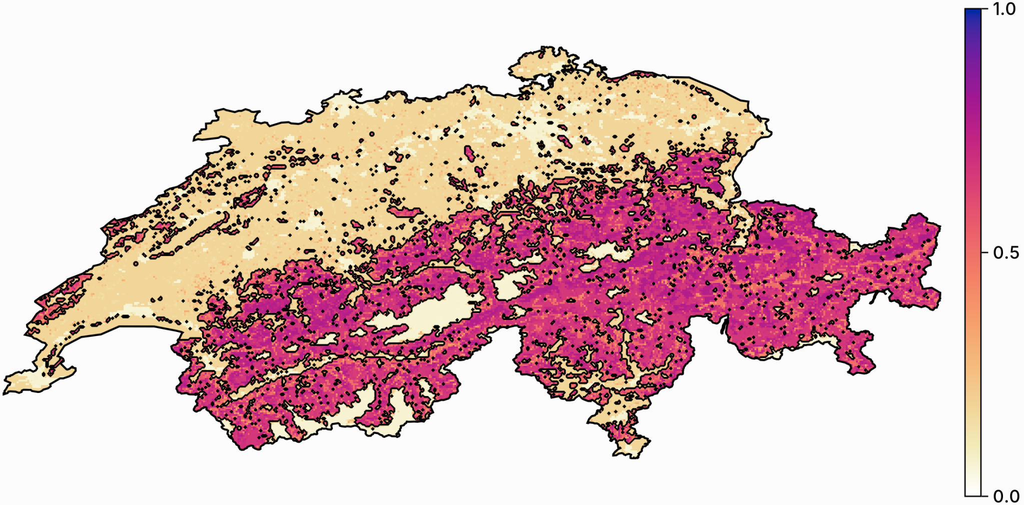
LIMITS OF A SINGLE MODEL

- a single model
- different parts of data may have different signal
- do we need all the variables all the time?
- bias v. variance tradeoff
- limit overfitting

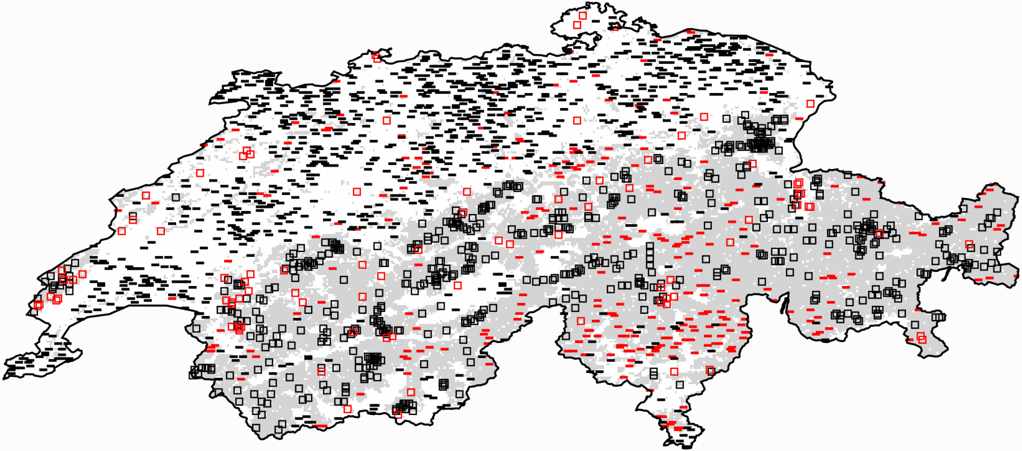
BOOTSTRAPPING AND AGGREGATION

AN EXAMPLE OF BAGGING: ROTATION FOREST

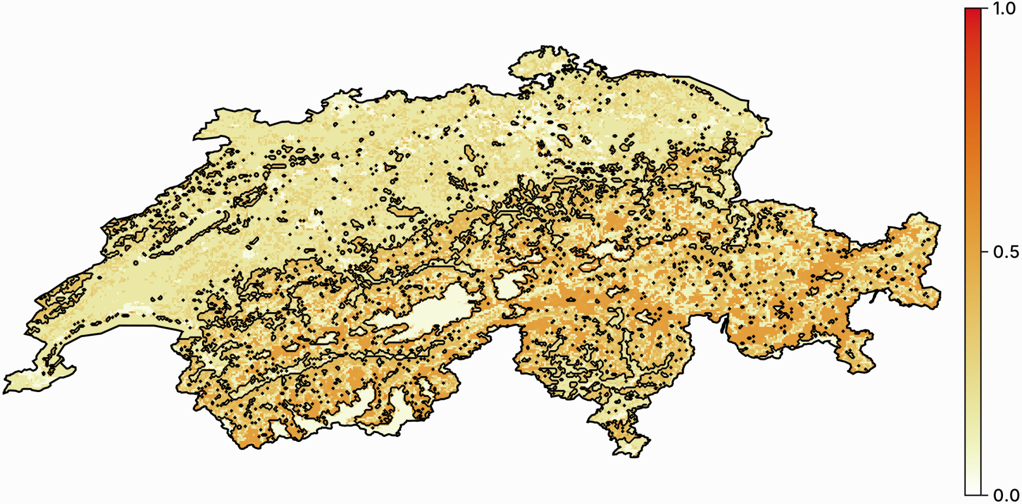
PREDICTION OF THE ROTATION FOREST



PREDICTION OF THE ROTATION FOREST



UNCERTAINTY



§ 6

Conclusions