

Method of AOA explained in figures

Supplementary to the paper ‘Predicting into unknown space? Estimating the area of applicability of spatial prediction models’

Hanna Meyer

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General problem of random forests in “unknown environments”

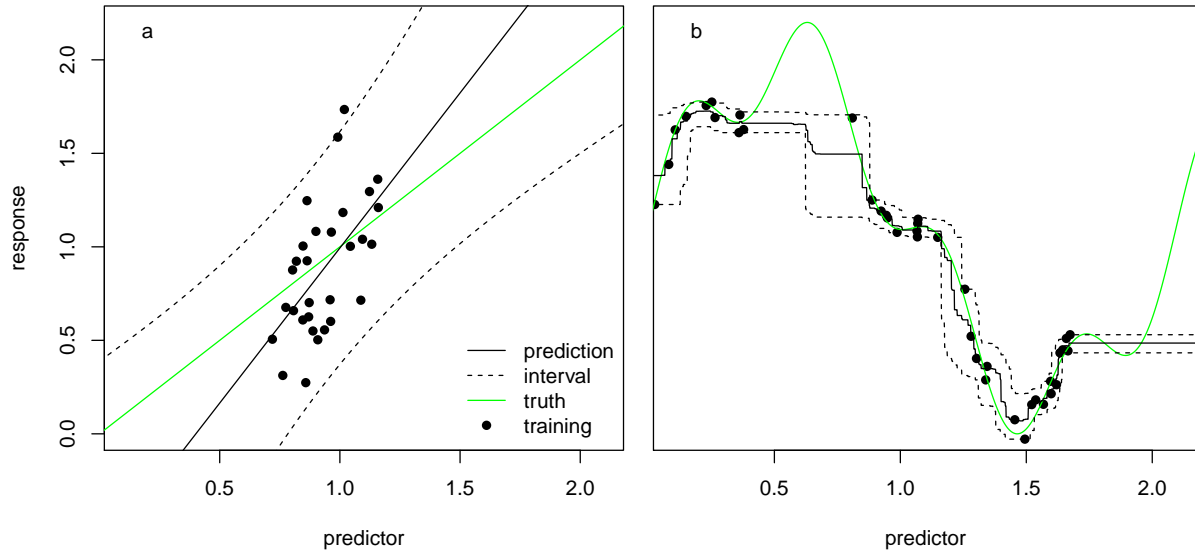


Figure 1: Problem of predicting beyond the training data and behaviour of prediction intervals for different models. Left: linear regression prediction interval width increases with distance from the center of the training data, right: a more complex relationship fitted with Random Forest. Prediction beyond the training data becomes highly unreliable, although prediction interval width outside the data range is constant. Random Forest prediction intervals were obtained by computing quantiles over the predictions from individual trees.

Method

Create Sample data, scale and weight them

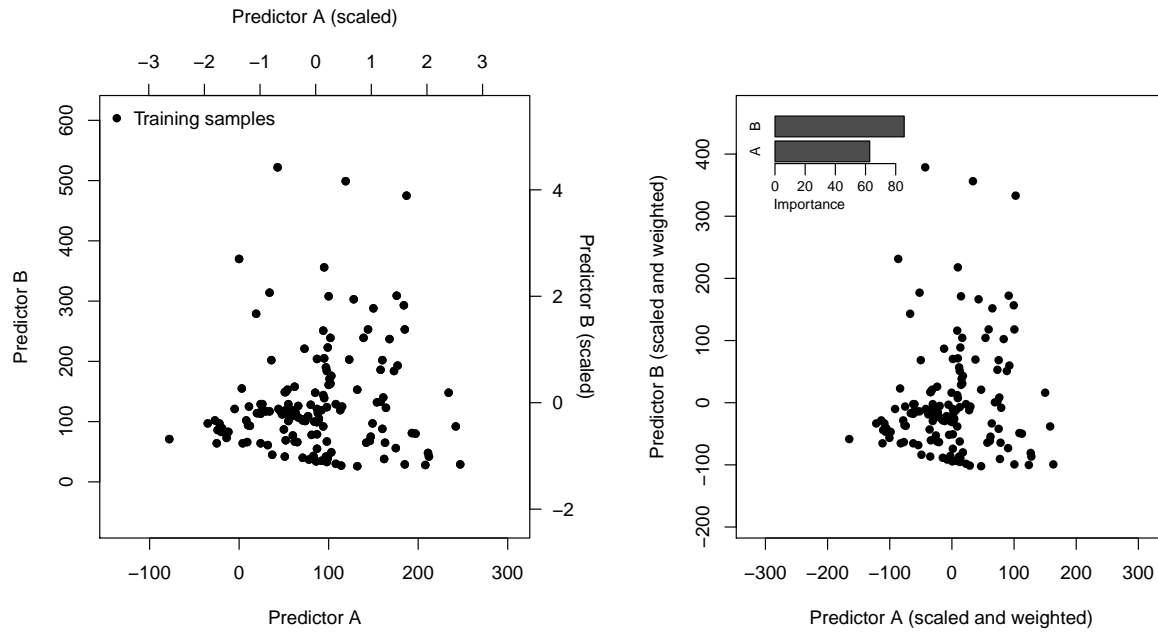


Figure 2: Initial situation: Training samples in a multidimensional (here 2) predictor space (a). First, the predictor space is scaled (second x and y axis in the left plot) and then and weighted (plot right) according to the estimated variable importance shown in the topright corner.

Calculate the DI within the training data to get the threshold for the AOA

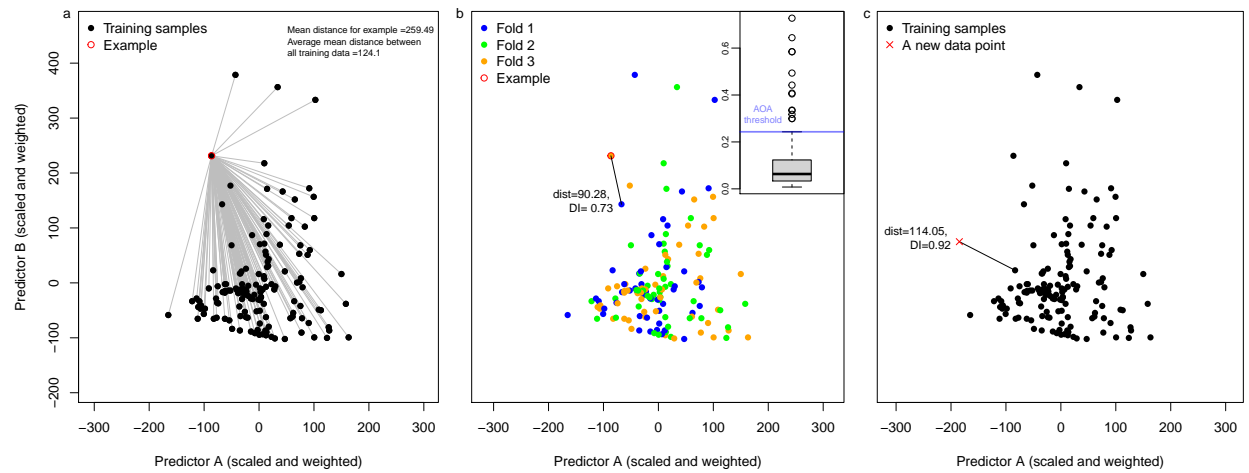


Figure 3: To answer the question if the trained model can be applied to a new data point, a threshold is used. This is the outlier-removed maximum DI of the cross-validated training data. The calculation of the DI of the training data is shown here for one example: The example data point is in fold 3 of the model. Therefore the distance to the nearest training data point NOT located in fold 3 is calculated (b) and this distance divided by the average of the mean distances between all training data (a). The DI is calculated for each training data point (boxplot) and the threshold is then derived from these DI values, so that a new data point (c) is outside the AOA if it is more dissimilar than the dissimilarity observed within the training data.

Estimate the AOA for each new potential data point

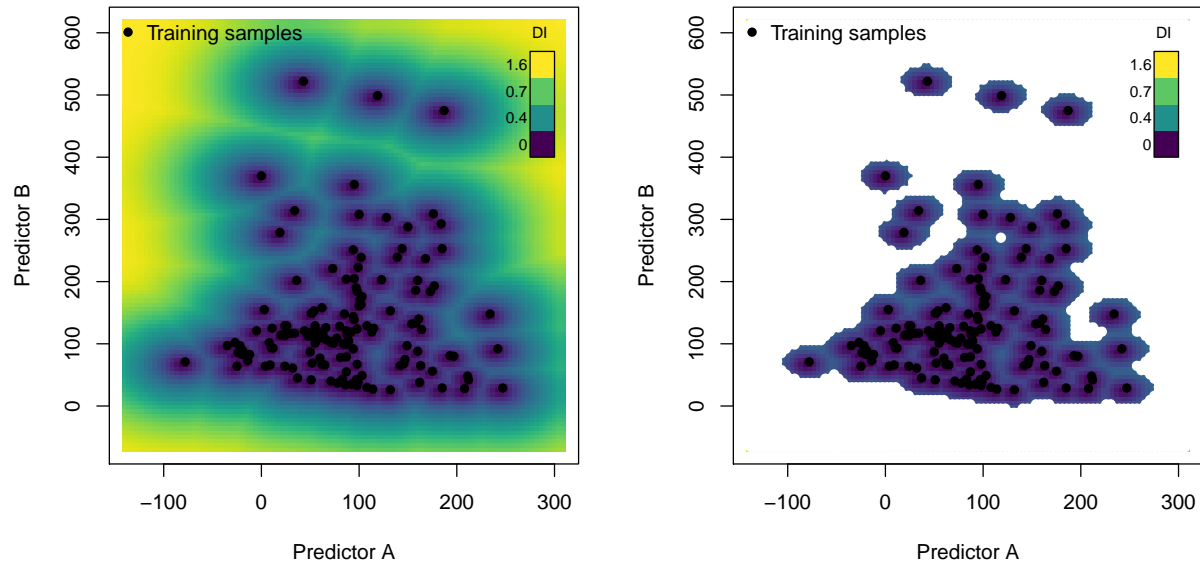


Figure 4: The AOA threshold can be applied to the entire predictor space to derive the AOA (b) from the DI (a) of each new data point.

Using the performance~DI relationship to get a quantitative uncertainty measure

Estimating the relationship using the cross-validated data

Relationship between the DI and RMSE based on the cross-validation folds used during model training and validation. RMSE was calculated in a sliding window of 10 along the DI. To estimate the RMSE based on the DI, a shape constrained additive model was used.

```
pdf("../figures/concept_figures/AOA_calib_singleCV.pdf",width=10,height=7)
singleCVAOA <- calibrate_aoa(newdat_aoa,model>window.size = 10)
invisible(dev.off())
```

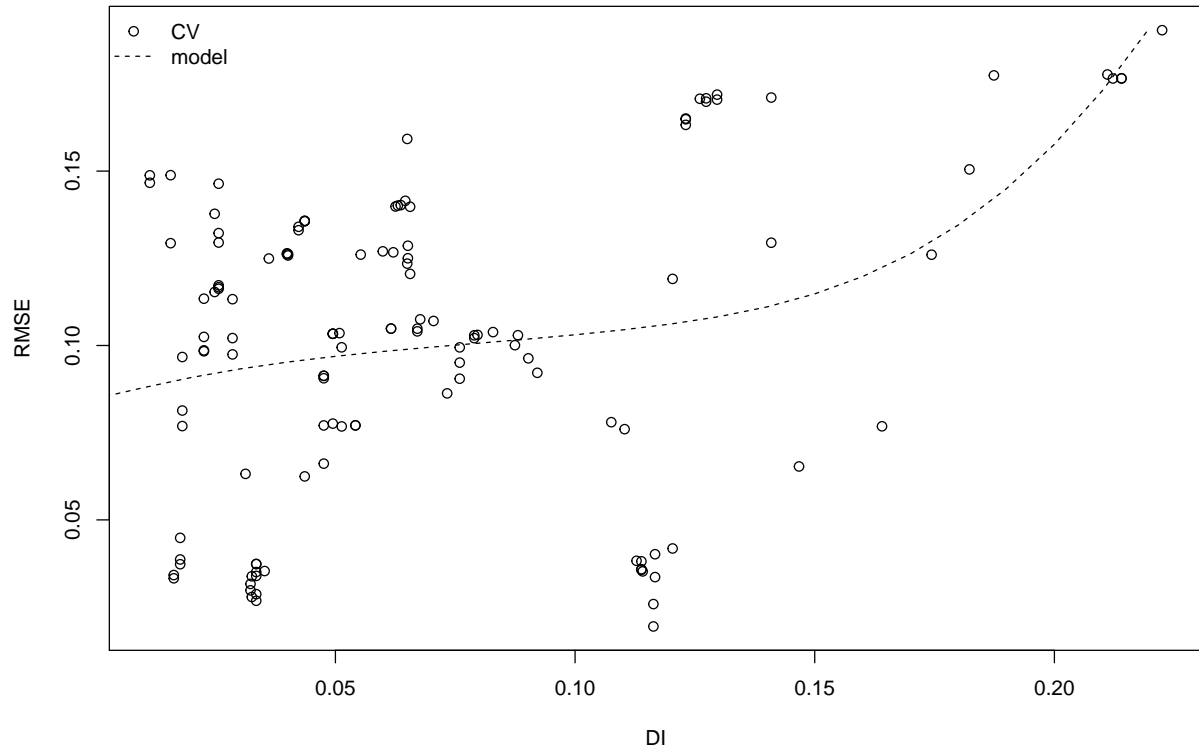


Figure 5: Relationship between the DI and RMSE within the AOA based on single cross-validation. RMSE was calculated in a sliding window along the DI. To estimate the RMSE based on the DI, a shape constrained additive model was used. Note that in this small example there is no strong relationship between DI and RMSE.

Using Multi-purpose CV

The results shown above are based on a single-purpose CV. We can also estimate the relationship between performance and DI using multiple CVs. Here, we split the data several times into folds using clusters in the predictor space with the number of clusters ranging between 3 and the number of data points (=LOOCV). The following figure shows how data splitting can look like for different numbers of k .

```
## pdf
## 2
```

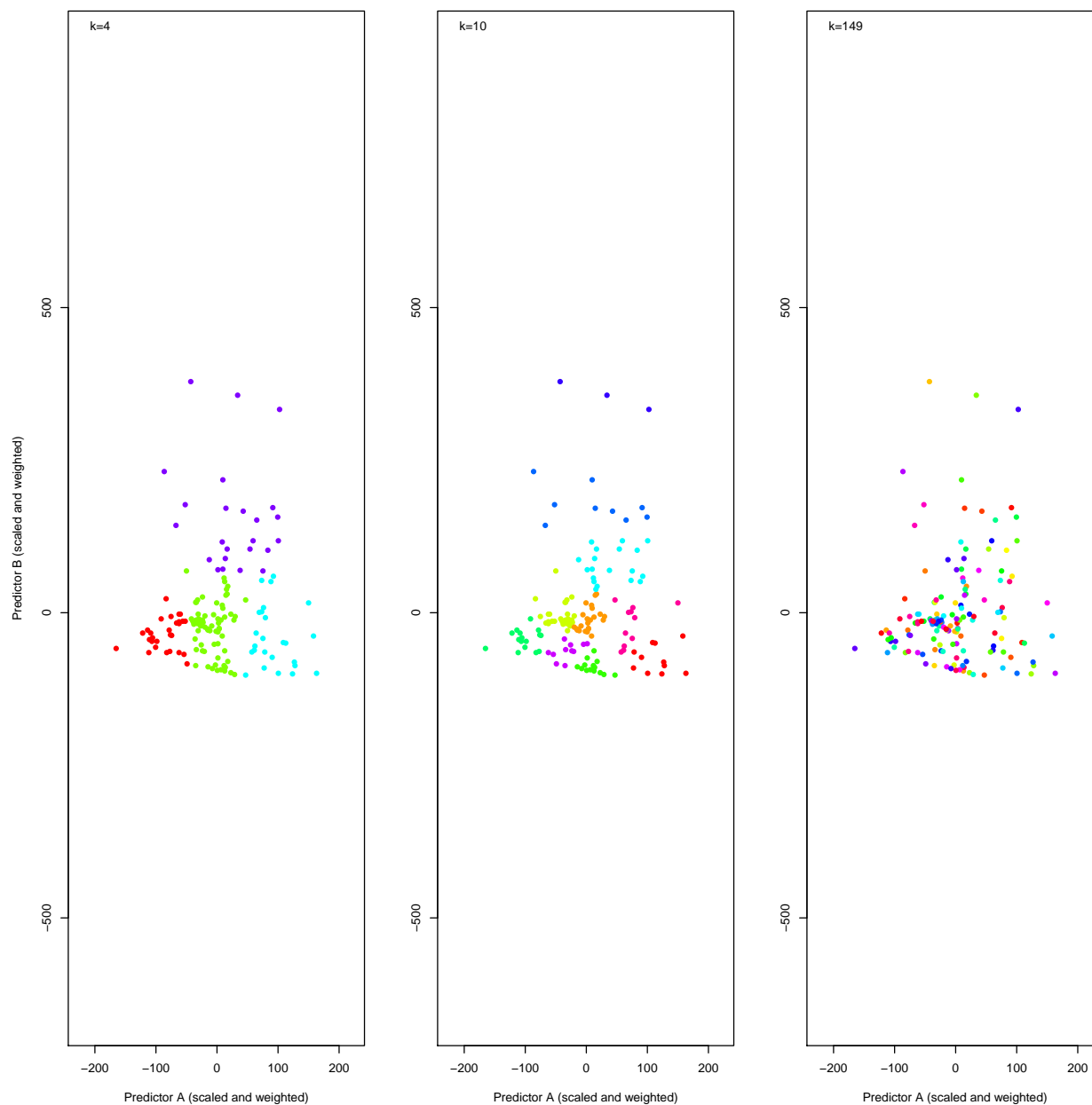


Figure 6: Example of multi-purpose cross-validation folds that have been assigned based on clusters in the predictor space.

Using multi-purpose CVs allows expanding the AOA and also allows giving a more robust estimate for the relationship. The relationship can be used to estimate the error for each new data point based on the DI.

```
pdf("../figures/concept_figures/AOA_calib_multiCV.pdf",width=10,height=7)
multiCVAOA <- calibrate_aoa(newdat_aoa,model>window.size = 25,multiCV = TRUE)
invisible(dev.off())
```

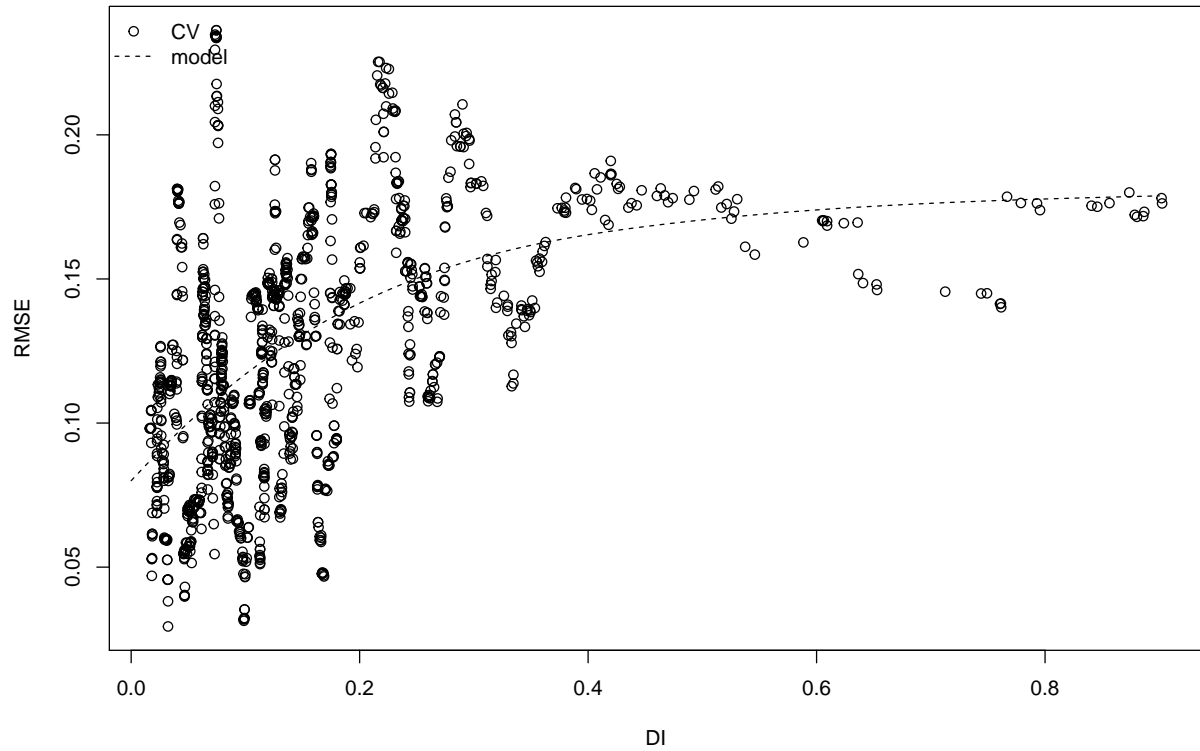
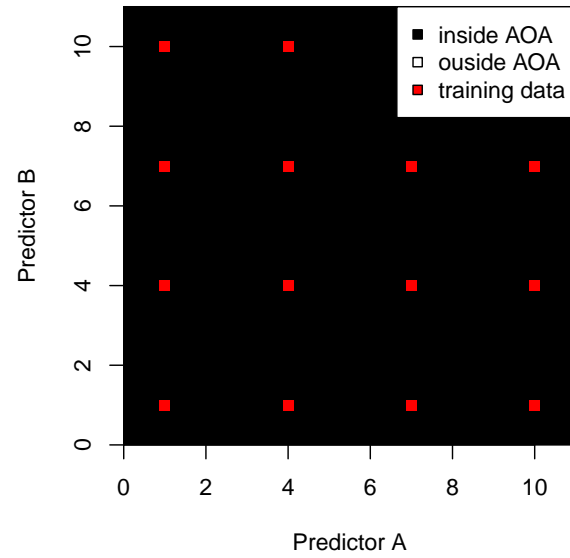
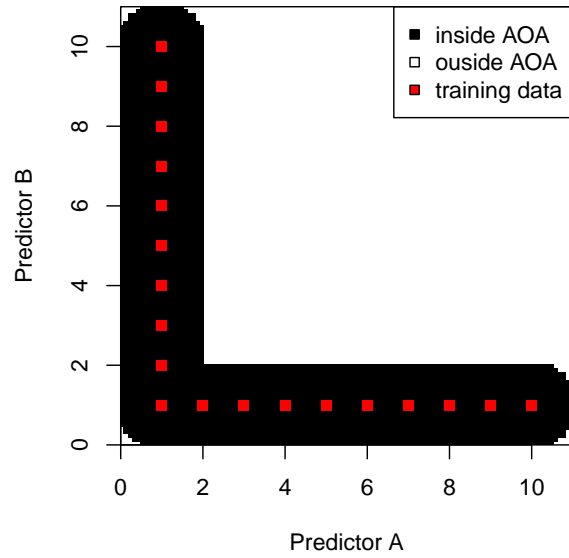


Figure 7: Relationship between the DI and RMSE within the AOA based on multi-purpose cross-validation. RMSE was calculated in a sliding window along the DI. To estimate the RMSE based on the DI, a shape constrained additive model was used. Note that in this small example there is no strong relationship between DI and RMSE.

FAQ explained in figures

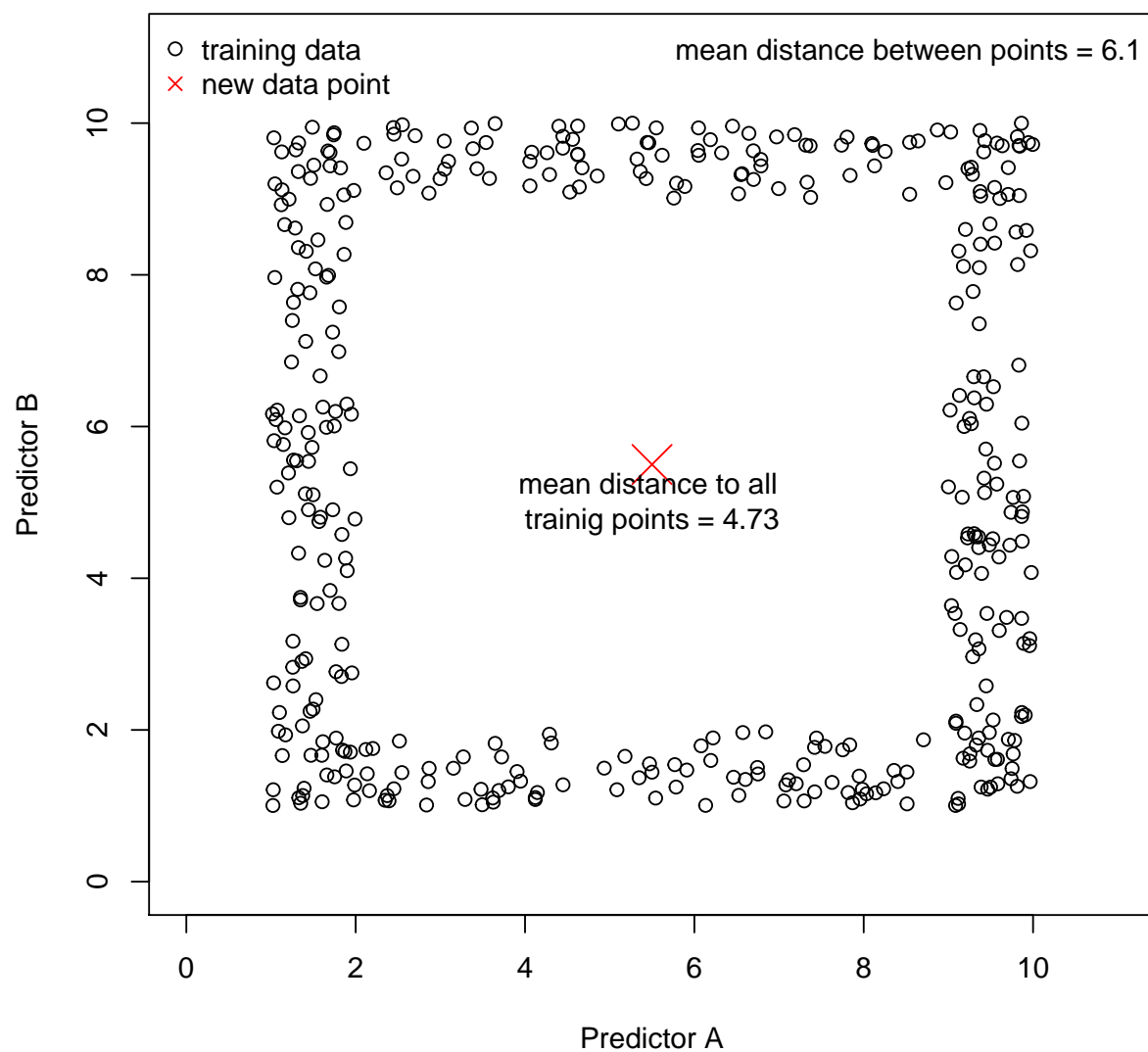
What happens if the full range of predictors is covered by training data?

When the full range of environmental conditions is covered the result is that the model can be applied to the entire study area. However, covering the full range of each variable is not enough (figure left) but the combined ranges need to be covered if the model should be applicable to the entire study area (figure right).



Why can't we use the distance to all data points instead of distance to the nearest neighbor?

The distance to all training points is not helpful here because then gaps could not be considered. But gaps are equally problematic (see our first figure in the manuscript) and using the average distance to training points cannot account for that. In the example below the new data point even has a lower average distance to training data although it is clearly in an area not covered by training data.



How would the AOA look like for Fig. 1 of the manuscript?

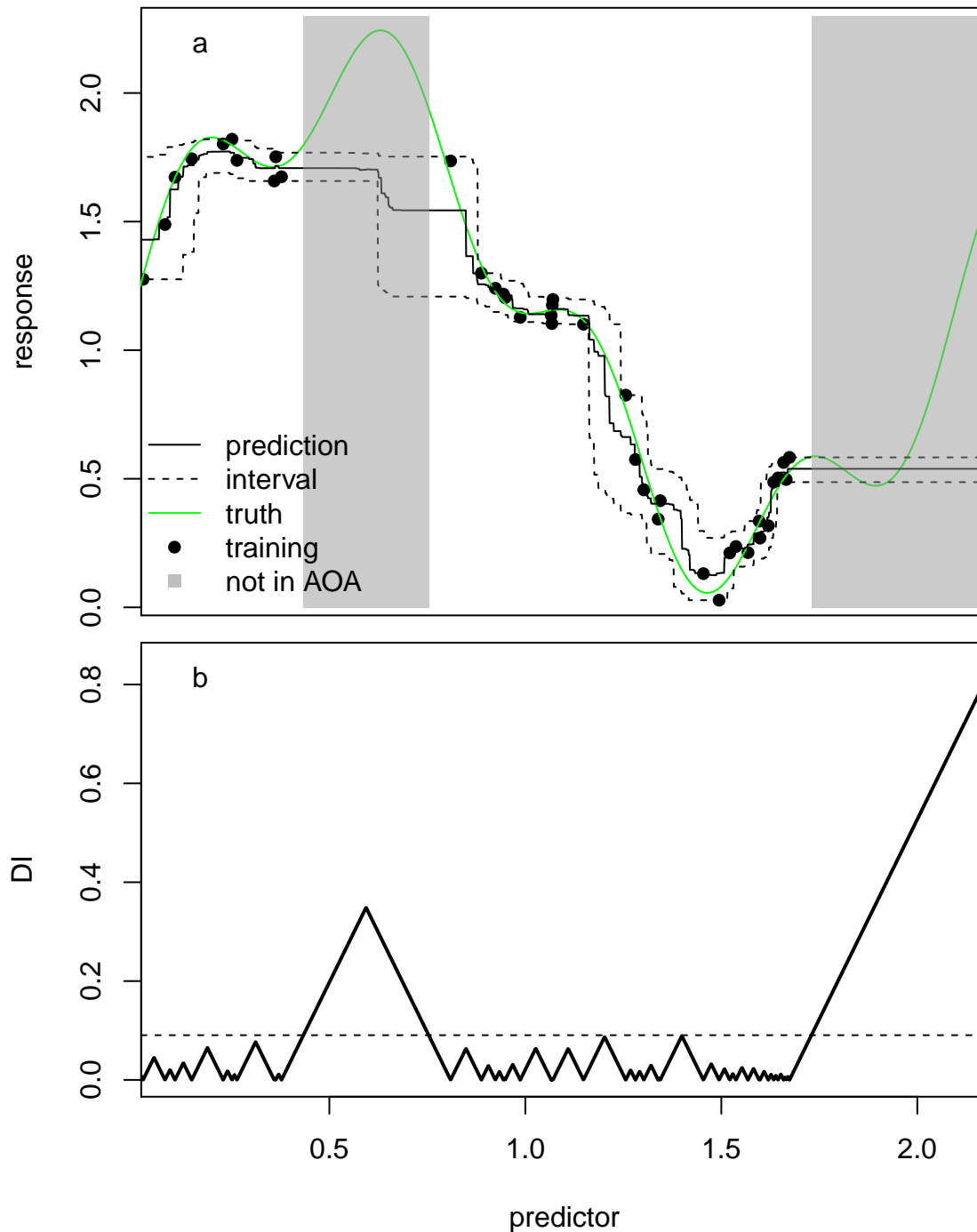


Figure 8: Hypothetical example of a relationship between a virtual predictor and response variable as well as the predictions made by Random Forest already presented in Figure 1. Low values in the dissimilarity index (DI) do not necessarily mean that the prediction error is high. As moving away from the last training data point ($x = 1.7$), the value of the DI increases (b). However, the error does not necessarily increase in the same way (comparing the predictions with the truth in a). The uncertainty must still be considered as very high because this area of the predictor space is unknown to the model. The area of applicability (AOA) is derived using the outlier-removed maximum DI observed in the cross-validated training data as a threshold (dashed line in b) and is used to exclude predictions in areas where dissimilarity is too high (grey area in a).