Bern University of Applied Sciences

Mastering Machine Learning for Spatial Prediction II

Model selection and interpretation, uncertainty

OpenGeoHub Summer School
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Madlene Nussbaum

Objectives ...

- Know **2** ways of ...
  - of **model selection**
  - of **model interpretation**
  - computation of **uncertainty**

- Learn why we do model selection (or not)
- Learn that **ML != black box**
- Learn why we need uncertainty and how to validate your prediction intervals

Overview

Model Selection

- linear regression
- with lasso
- with covariate importance

Model interpretation

- partial residual plots
- partial dependence plot
- partial dependence maps

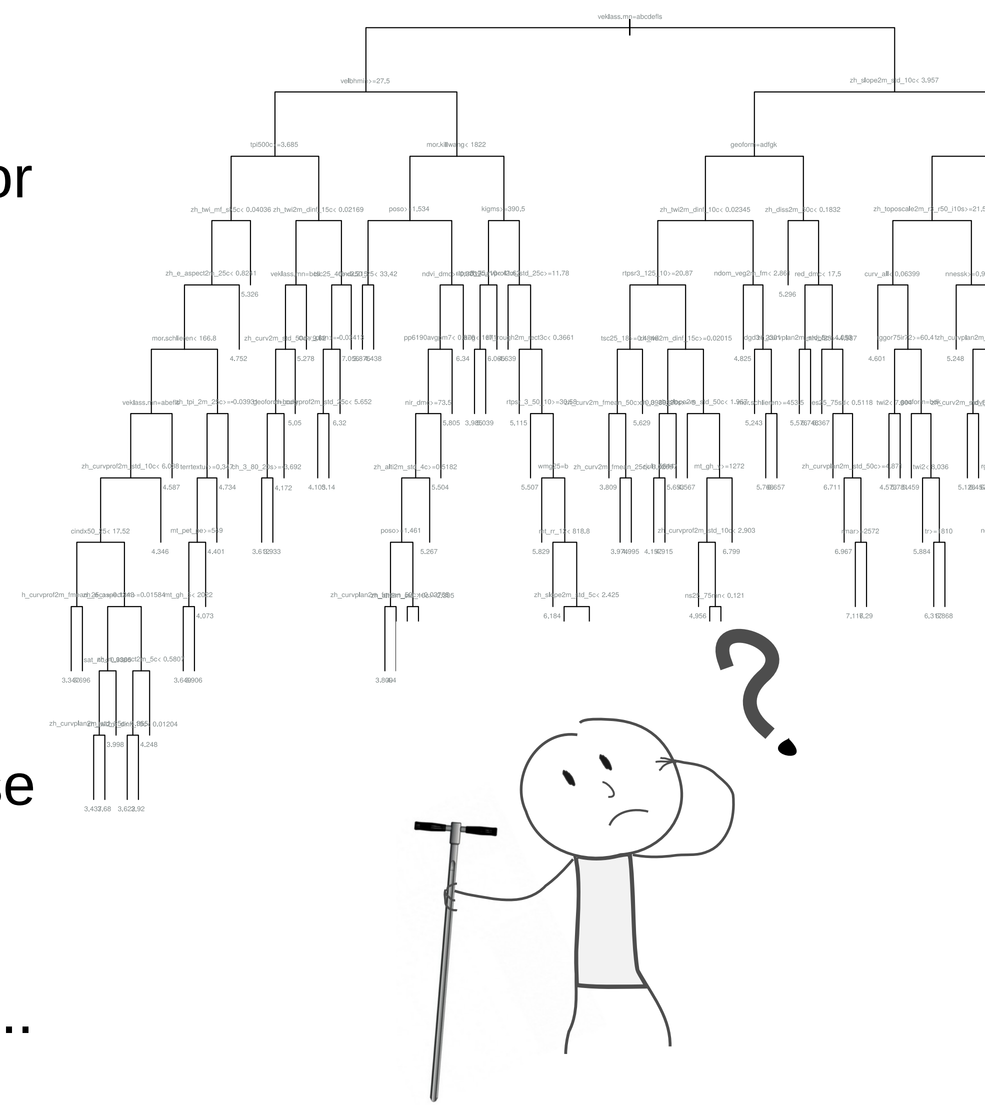
Uncertainty

- non-parametric bootstrap
- model-based bootstrap
- evaluation

Is there a reason for model selection? Or is it enough to do model building?

Model selection = reduce the inital covariate set
Model building = find relationships between covariates and response

- ✔ Model interpretation
- ✔ Better just use relevant covariates for prediction
- ✔ Computational effort for predictions
  (just prepare 12 instead of 300 rasters)
- ✔ Maybe reduce effort for future data collection and modelling on same topic
- ✖ However, theoretical statisticians do not recommenced selection, because it is often biased, difficult to find the true model..
- ✖ We might loose prediction accuracy...



Model flexibility vs. model complexity

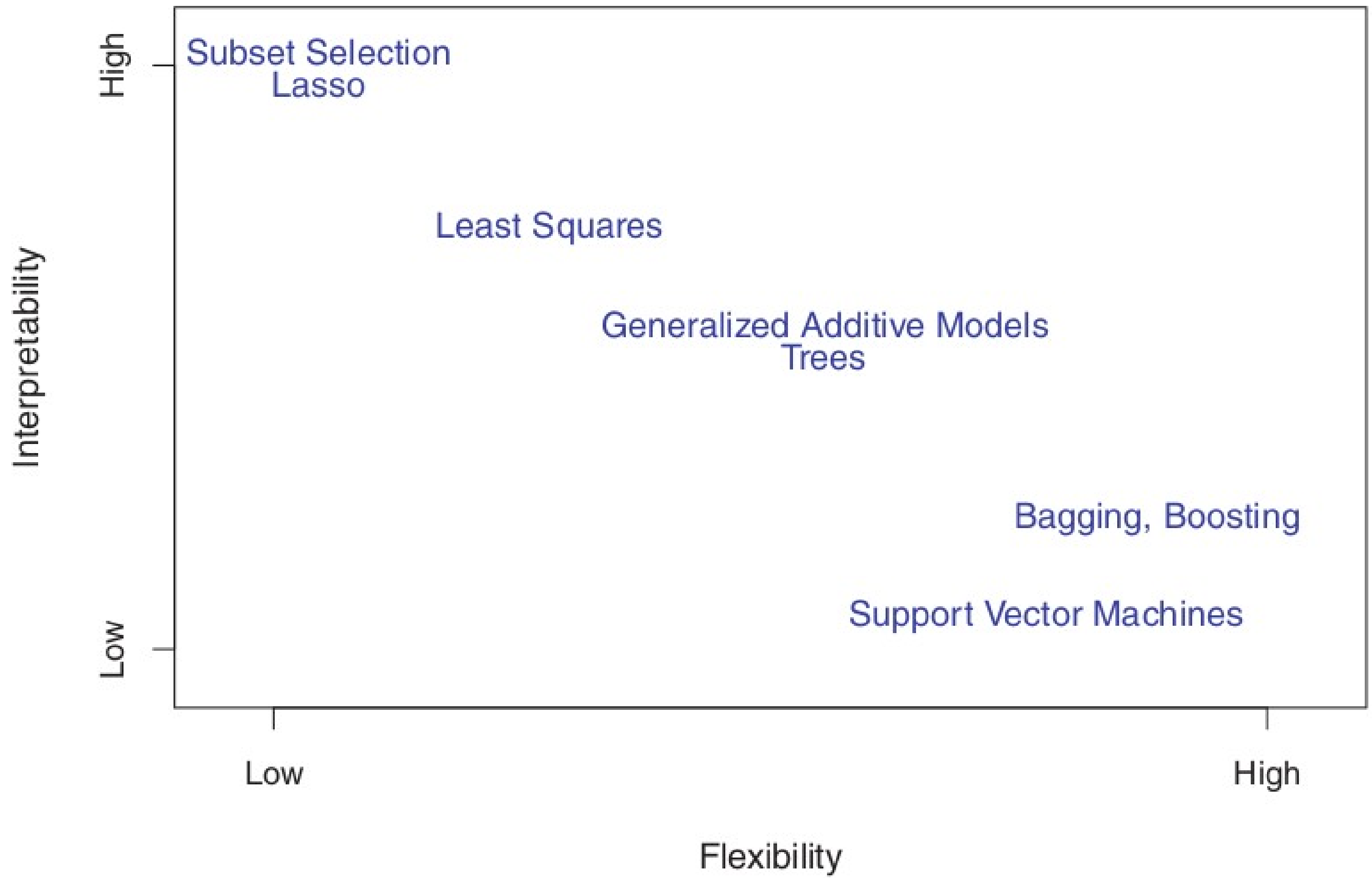
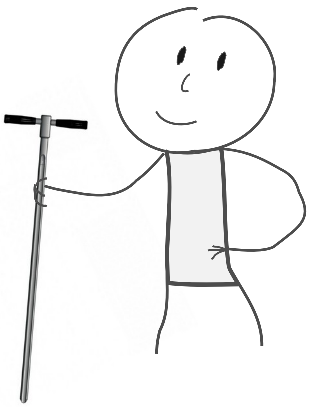


FIGURE 2.7. *A representation of the tradeoff between flexibility and interpretability, using different statistical learning methods. In general, as the flexibility of a method increases, its interpretability decreases.*

Gareth et al. 2013, p. 25

Model selection – strategies



- Ask a domain expert that is familiar with the topic of your modelling problem
- Remove *n* worst covariates
- Stepwise addition or removal (see later)
- Test all possible models
- Shrinkage (e.g. by boosting or lasso, see later).

Model selection for linear regression

Usually used for linear models (e. g. OLS):

- Forward selection
  - Start with a model with just an intercept
  - Try all possible covariates and add the one that results in the best fit (e.g. R^2)
  - Add covariates until increase in R^2 is only very small (threshold) or evaluate the gained models by cross validation.

- Backward elimination
  - Fit the full model with all covariates
  - Remove the covariate that will cause the smallest decrease in R^2
  - Continue removing until the drop in R^2 gets too big (threshold) or evaluate the fitted models by cross validation

Model selection for linear regression

Evaluation of forward and backward selection:

- ✔ Straightforward, easy to understand
- ✔ Follows a selection path, hence much more efficient and less arbitrary than best subset selection
- ✖ Binary selection: A covariate is either in or out.
  Being in by e.g. 30 % is not possible.
- ✖ Multi-collinearity, unstable fits!
  We need to remove correlated covariates beforehand.
- ✖ Likely overfits the data, biased model selection.
  Most often does not find true model.
- ✖ We can not fit p > n

→ Possible solution: regularization / shrinkage with e.g. **lasso**.

Model selection with lasso

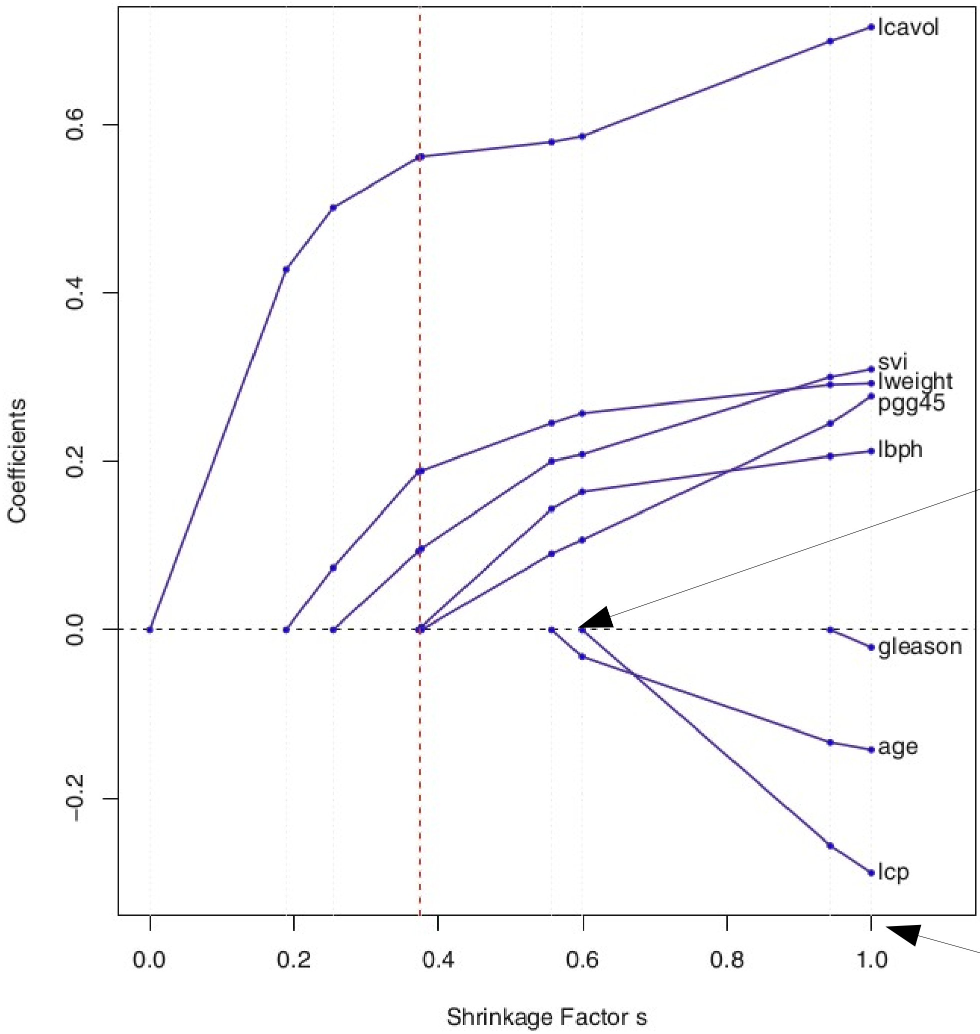


FIGURE 3.10. *Profiles of lasso coefficients, as the tuning parameter t is varied. Coefficients are plotted versus $s = t/\sum_1^p |\hat{\beta}_j|$. A vertical line is drawn at $s = 0.36$, the value chosen by cross-validation. Compare Figure 3.8 on page 65; the lasso profiles hit zero, while those for ridge do not. The profiles are piece-wise linear, and so are computed only at the points displayed; see Section 3.4.4 for details.*

Hastie et al. 2009, p. 70

Path of coefficients for increasing tuning parameter

Coefficient becomes 0, meaning the covariate is removed from the model

With lambda = 1, there is no shrinkage, and we have the normal ordinary least squares linear model fit

Covariate selection for random forest
(or boosted trees)

What again was this **out-of-bag (OOB) error**?

For each observation $z_i = (x_i, y_i)$, construct its random forest predictor by averaging only *those trees corresponding to bootstrap samples in which z_i* did not *appear.*

Hastie et al. 2009, p. 593

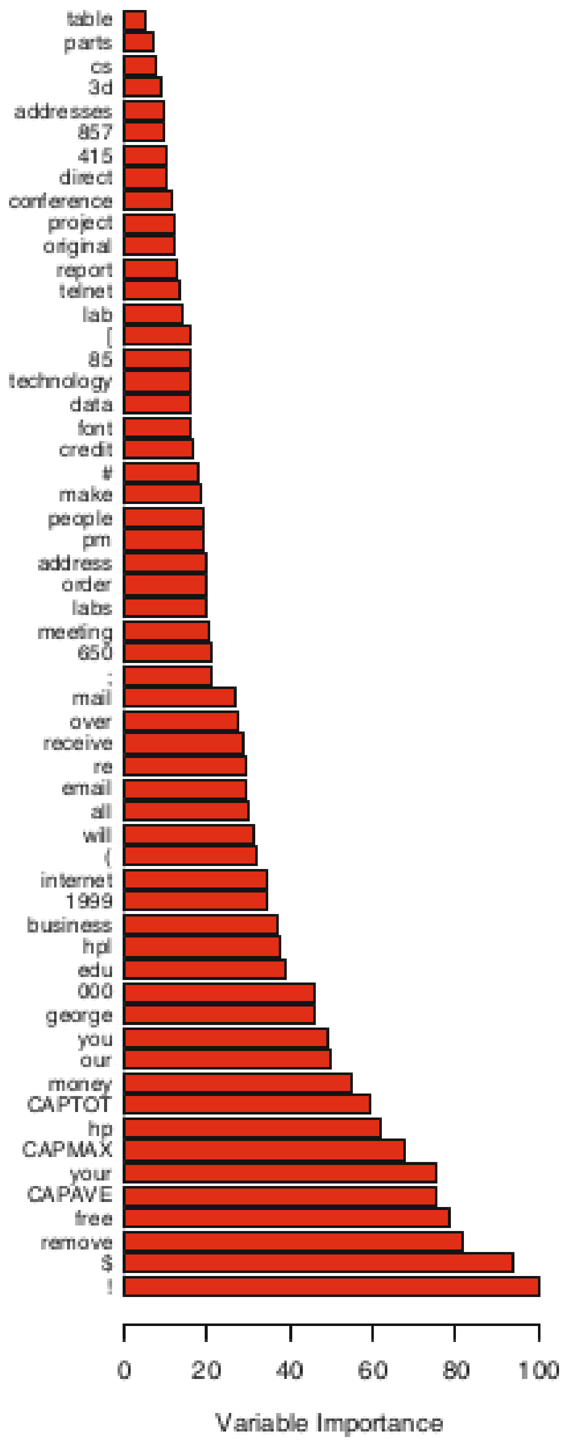
2 types of covariate importance:

- Sum of decrease in goodness-of-fit error by adding splits of this covariate (impurity), oriented on fitting the data. How much do we reduce error by using this covariate at this split?

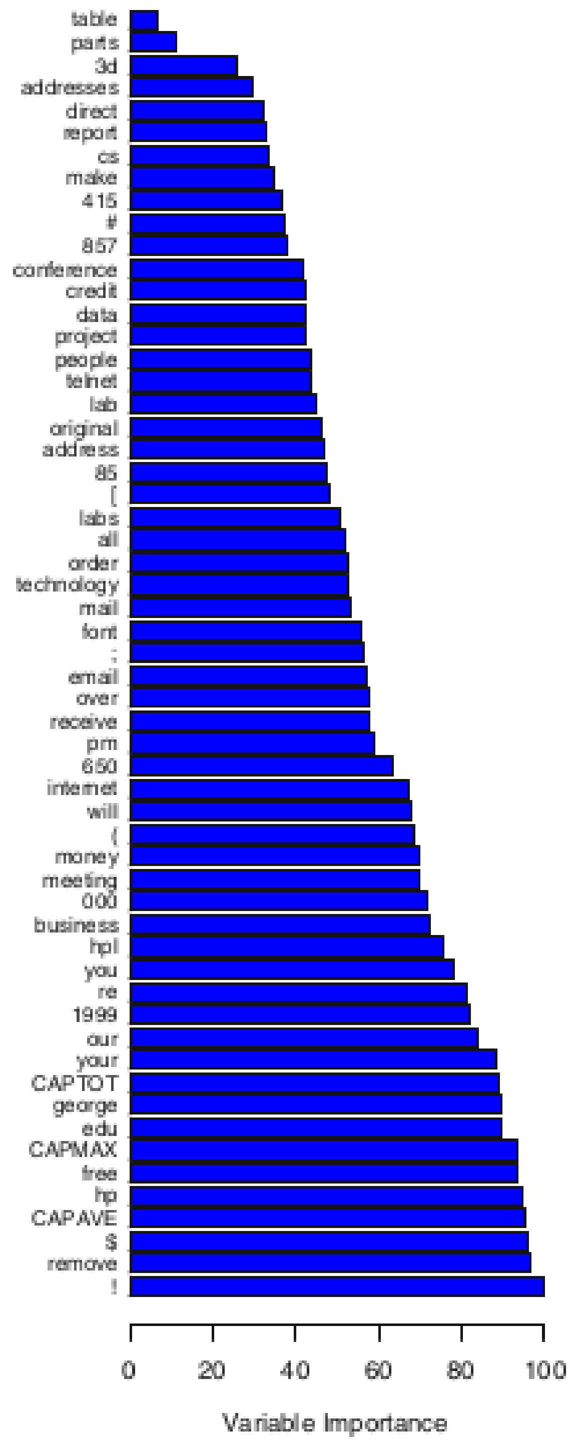
- Mean decrease in OOB error by randomly permuting a covariate, oriented on predictions.
  How much worse do OOB predictions get if we randomly shuffle a covariate?

  → removing a covariate is not the same, other correlated covariate could replace its “predictive capacity”

Loss in accuracy



OOB, Permutation



Hastie et al. 2009

Selection, very simple:

Recursive backward elimination

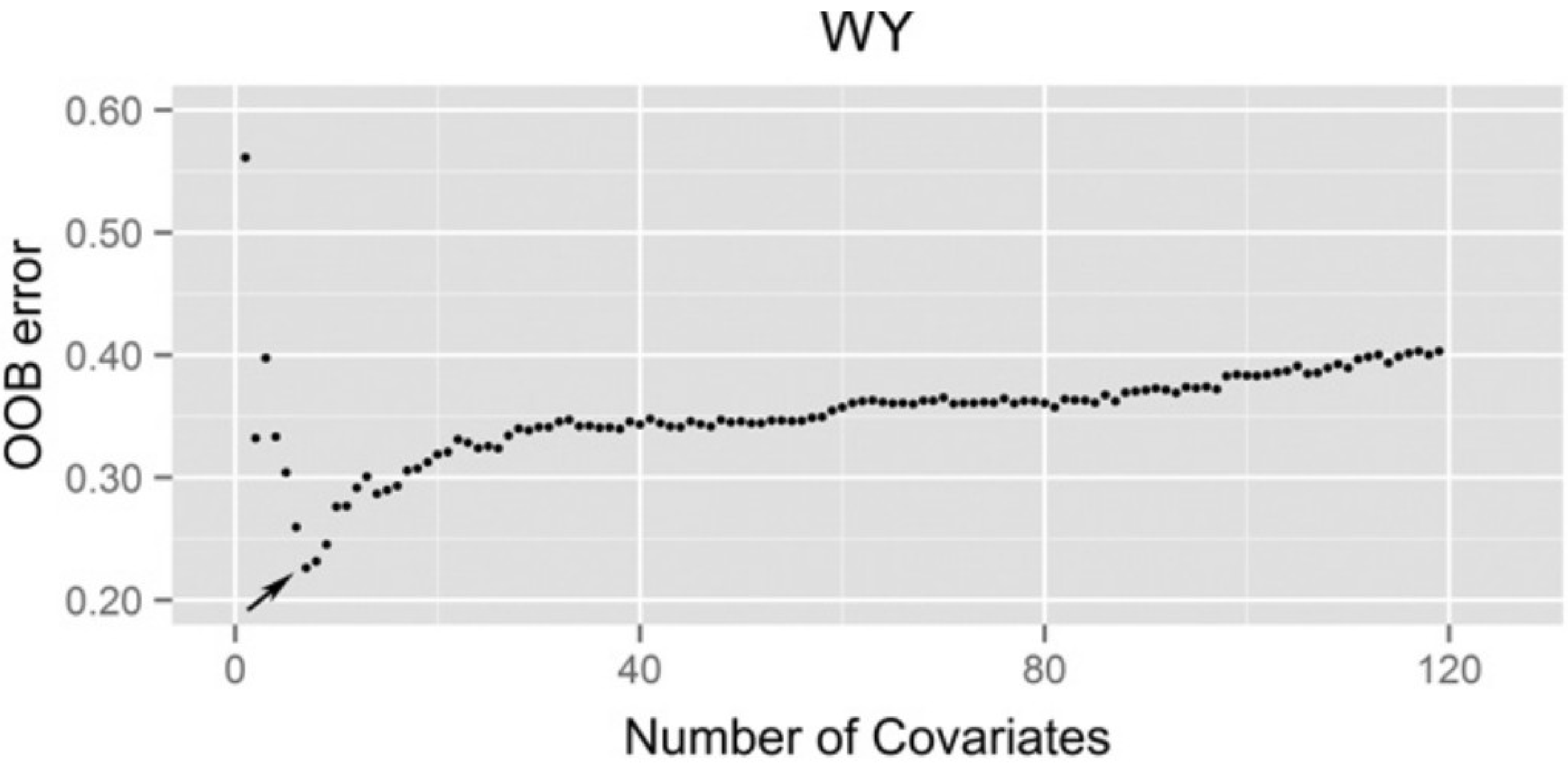
1) Remove covariate(s) with lowest importance

2) Refit random forest with remaining

Find optimum number of covariates by minimizing OOB error.

<u>Problem</u>:
Correlated covariates remain, because of randomisation at each split (m_{try}) . Interpretation needs to account for that.

Covariate selection for random forest
(or boosted trees)



Brungard et al. 2015

Model selection with random forest

- ✔ Straightforward approach
- ✔ Easy to implement
- ✔ From my experience: efficient
  (meaning a lot of covariates are removed)

- ✖ Correlated covariates remain in the model
- ✖ Artefacts in predictions possible
- ✖ Stability unclear?
  (Small changes in covariate or response values might change result drastically)
- ✖ Biased?
  (maybe biased as other backward elimination methods)
- ✖ Time consuming
  (iterative method, no paralell computing possible)
- ✖ Possibly: A lot of effort for a small result

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Covariate interpretation for any model

Partial residual plots (see e.g. Wikipedia)
Regression based methods, plot *Residuals* of full model plus the covariate effect $\hat{\beta}_i X_i$ against the values of covariate X_i

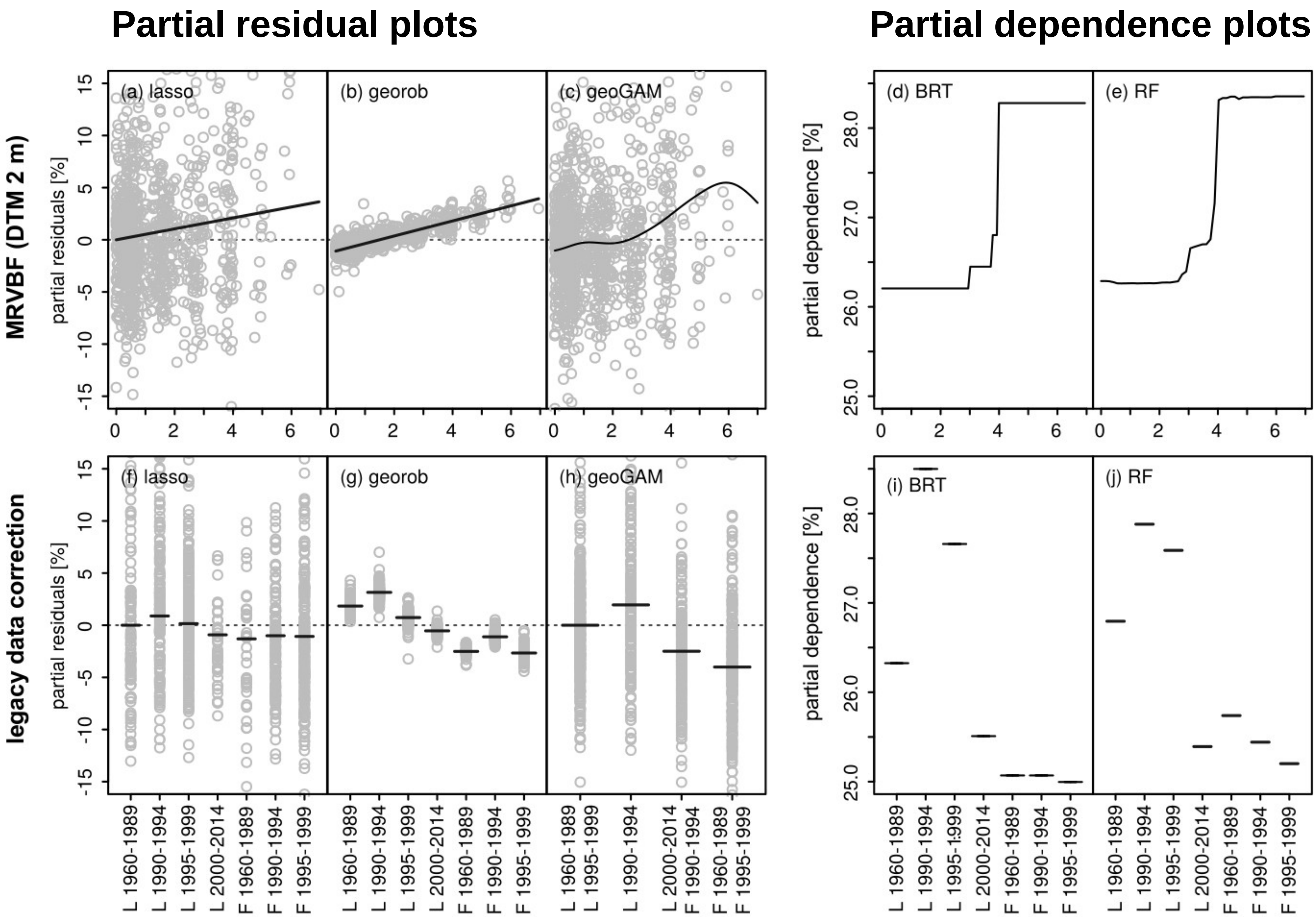
$$Residuals + \hat{\beta}_i X_i \;\; versus \;\; X_i$$

Partial dependence plots Hastie et al. 2009, chapt. 10.13.2
Any “black box” learning model, dependence of covariate on response after *accounting* (not *ignoring*) for the effects of all other covariates.
Approximation of function by:

$$\bar{f}_S(X_S) = \frac{1}{N}\sum_{i=1}^{N} f(X_S, x_{iC}),$$

Take care with interpretation: If many covariates it is difficult to choose which to interpret. If collinearity in data set, covariates might replace each other …

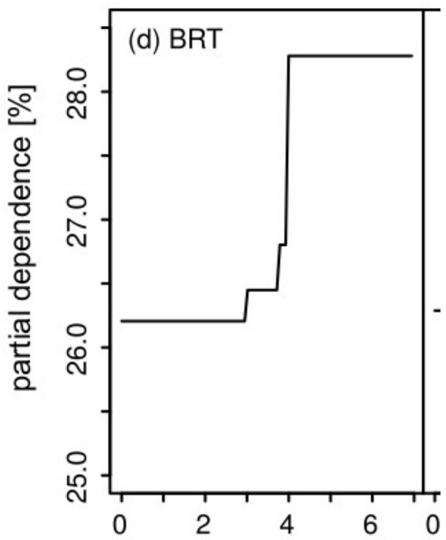
Covariate interpretation for any model

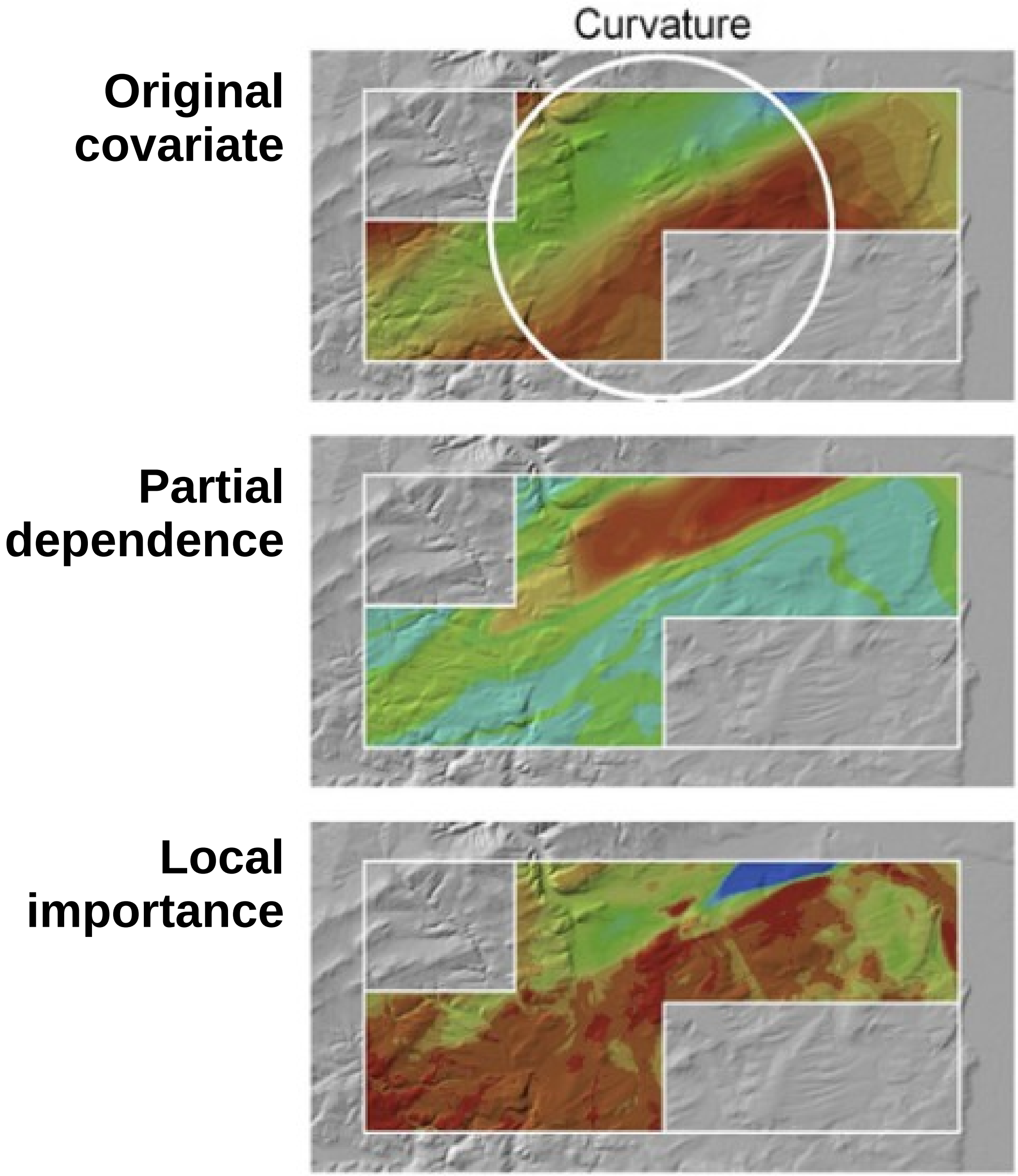


Nussbaum et al. 2017b

Spatial covariate interpretation

Create maps from relationship:





Behrens et al. 2014

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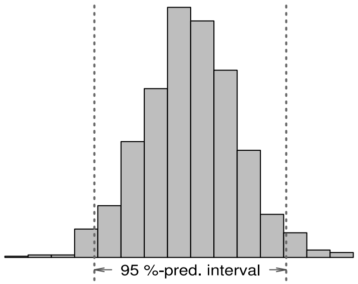


Confidence intervals vs. prediction intervals

Confidence intervals

Intervals of confidence for the estimate of a population mean. Considers uncertainty in our estimation of β (based on standard error of coefficient).

$$y = X\hat{\beta} + \epsilon$$

Prediction intervals

Intervals of confidence for the estimate of a new observation. Considers uncertainty estimated β and the variation the model does not account for (based on standard error of coefficient and residual error).

$$y = X\hat{\beta} + \epsilon$$

Non-parametric bootstrap – idea

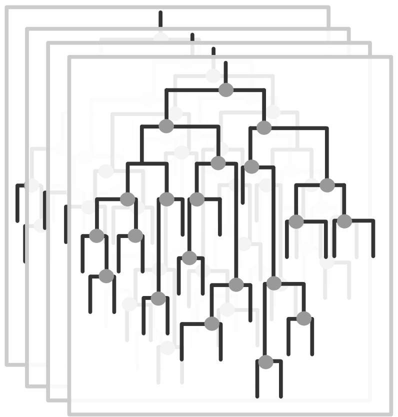
Total population
= sampling all the soil in the study area

Sample of population
= n soil profiles or soil cores

Sample of sample
= m soil profiles or soil cores ($n > m$)

Assumption
these relationships are the same

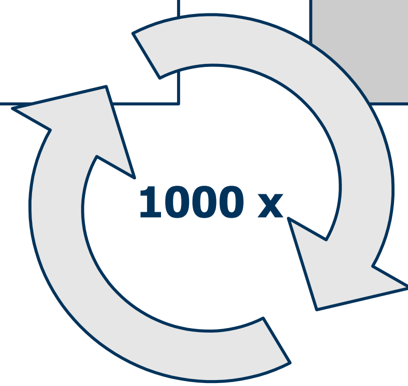
- Idea: by **resampling** our sample many times (e.g. 1000x) we can approximate properties of the **distribution** of the total population.
- Useful to
  - create model ensembles
    bagging = boostrap aggregation
  - estimate uncertainty for any model

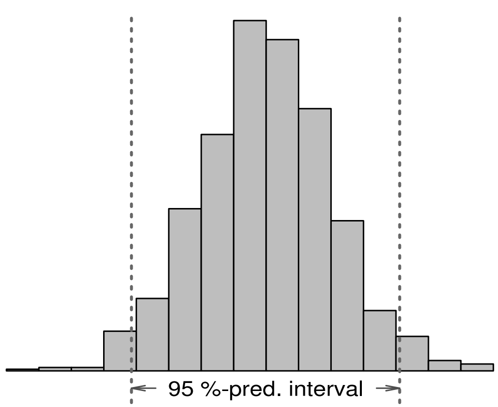


Simulate predictive distribution non-parametric bootstrapping ("model-free")

1. resample data with replacement to get a dataset with the same n

2. fit model to resampled data, compute predictions for new observations



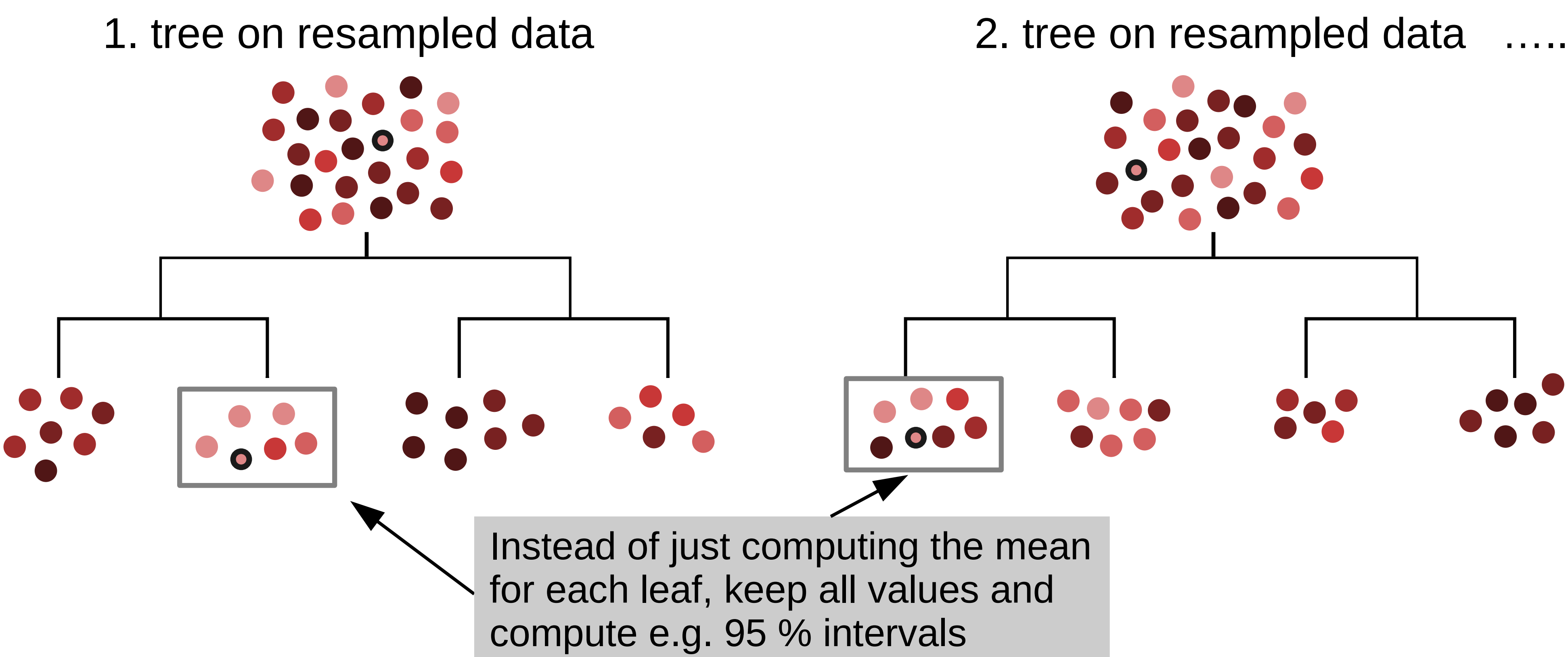


95 % prediction interval

“Quantile regression forest” as non-parametric bootstrap

Citation: Meinshausen N, 2006. Quantile regression forests. Journal of Machine Learning Research, 7, 983–999.

- Bootstrap aggregation in random forest: each tree is fitted to a resampled dataset
- Keep all observations in the final tree leaves
- Get distribution from observations that were in leaves together

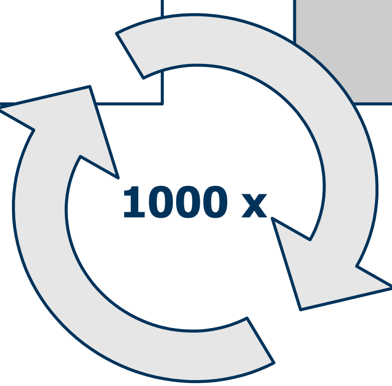


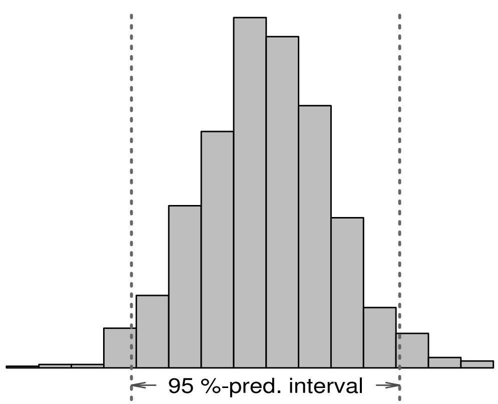
Simulate predictive distribution by <u>model-based</u> bootstrapping

1. simulate response under the final model

$$Y(s)=\sum f(X,s)+\epsilon$$

2. fit model to simulated response, compute predictions for new observations





95 % prediction interval

Model-based bootstrapping
(also “parametric bootstrap”)

Davidson and Hinkley, 1997

For 1000 repetitions, do:

1. Simulate new response *Y*(s)* with the fitted value *f(x(s))* plus a randomly chosen residual sampled from ε
   (or from normal distribution with same σ, μ as residual distribution):
   $$Y(\mathbf{s})^* = \hat{f}(\mathbf{x}(\mathbf{s})) + \epsilon$$

2. Fit model to new response *Y*(s)*

3. Compute prediction error for new location s+
   with again randomly sampled ε
   $$\delta_+^* = \hat{f}(\mathbf{x}(\mathbf{s}_+))^* - (\hat{f}(\mathbf{x}(\mathbf{s}_+)) + \epsilon)$$

Two-sided prediction intervals: $[\hat{f}(\mathbf{x}(\mathbf{s}_+)) - \delta^*_{+(1-\alpha)}\,;\ \hat{f}(\mathbf{x}(\mathbf{s}_+)) - \delta^*_{+(\alpha)}]$.

Which bootstrap should I use?

non-parametric

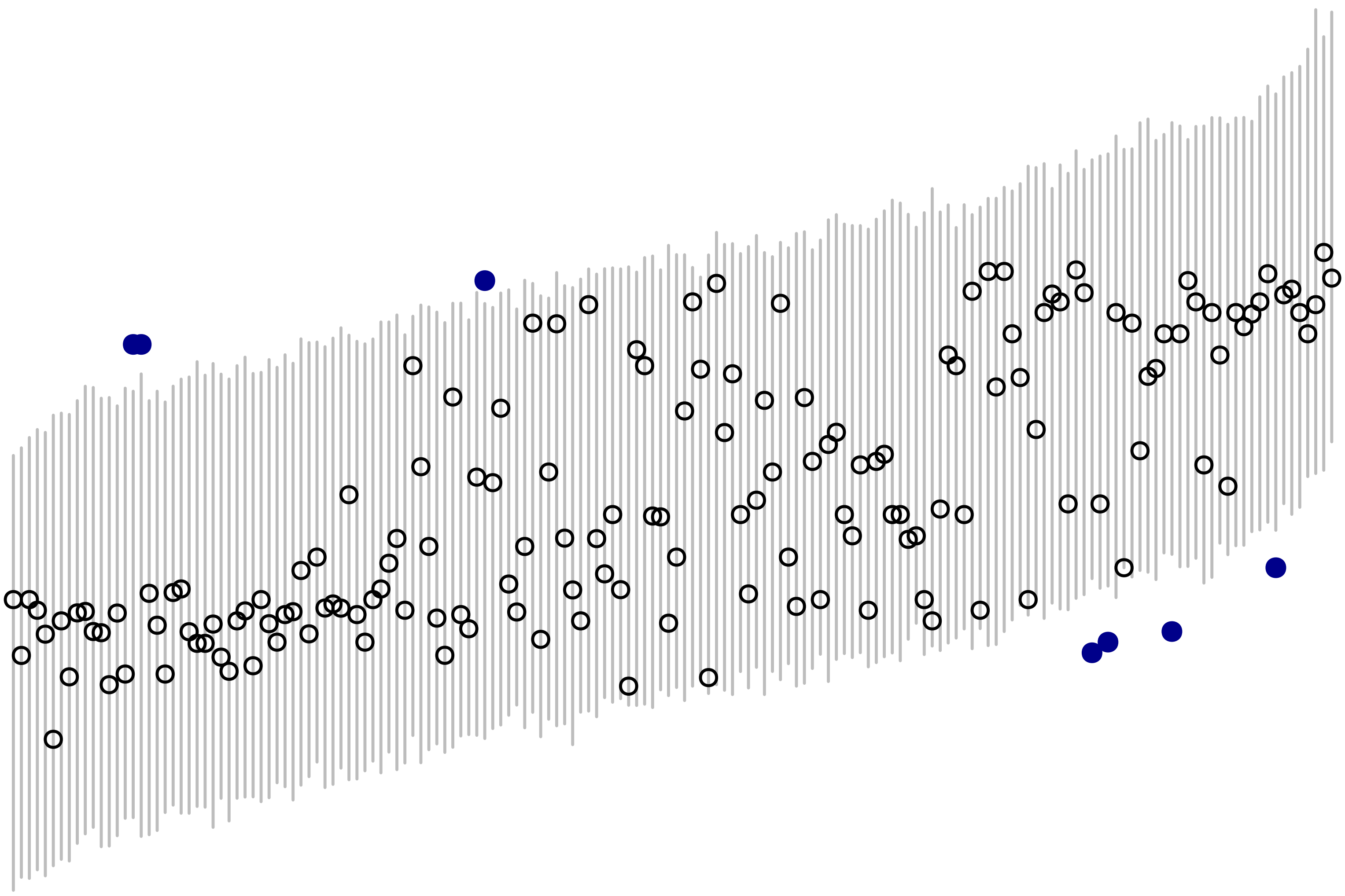
- ✔ No assumptions about a model or error distributions
- ✖ Likely to fail with small datasets:
  - underestimates variance
  - lacks to depict distribution of full population
- ✖ mostly no software
- ✔ easy to implement
- ✖ computationally intensive (mainly CPU)

model-based / parametric

- ✖ Assumes e.g. Gaussian errors
- ✖ Prediction intervals are given this model even if model is wrong
- ✔ More suitable for small datasets
- ✖ mostly no software
- ✖ a bit tricky to implement
- ✖ computationally intensive (mainly CPU)

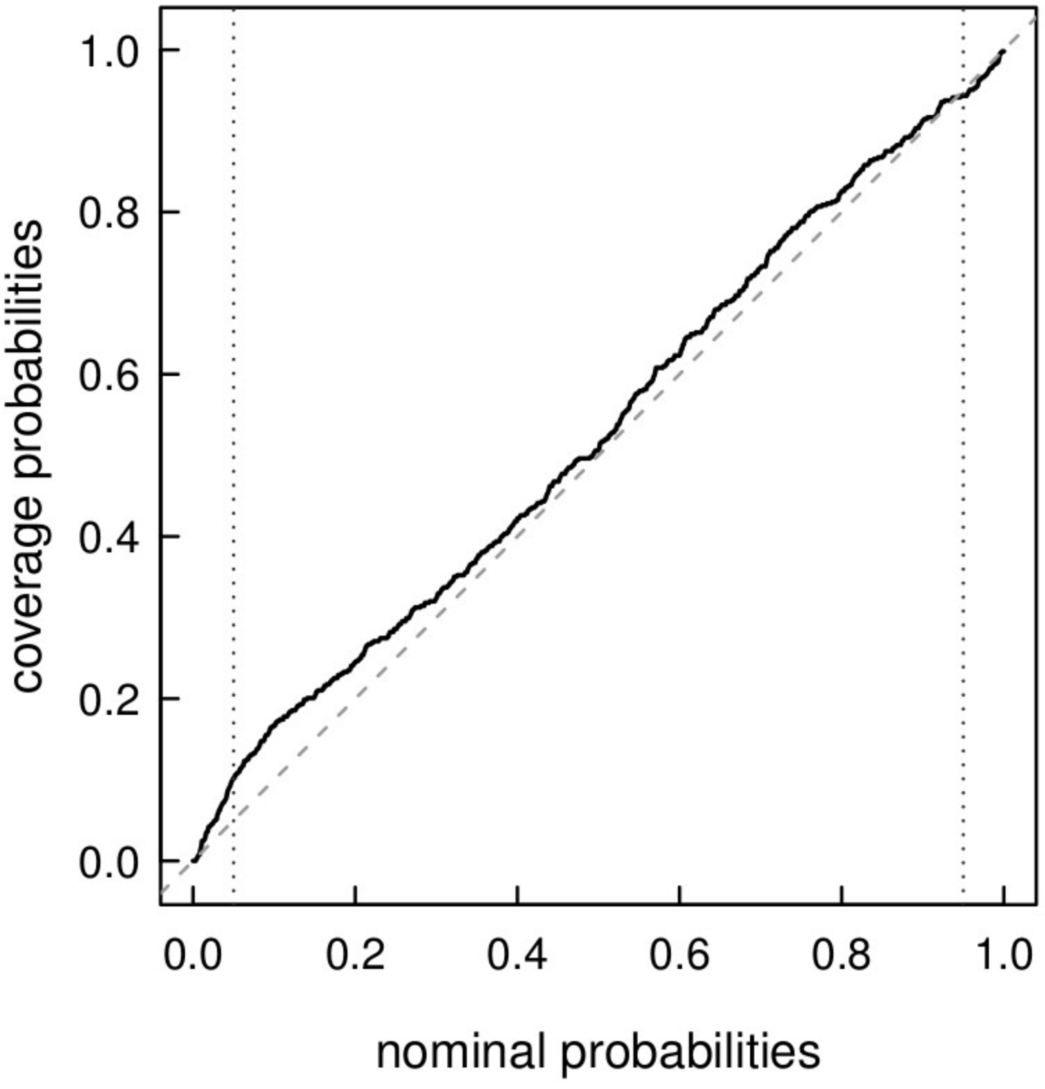
Performance plots for e.g. 95% prediction intervals

Evaluation with
independent
test data



Performance plots for complete predictive distribution

<u>one-sided</u> prediction intervals of bootstrapped distribution against the nominal probabilities

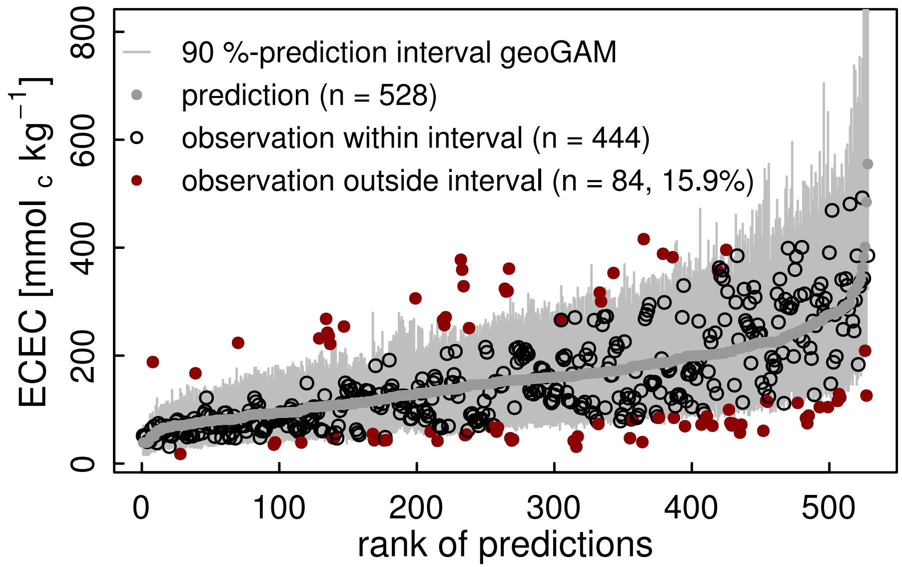


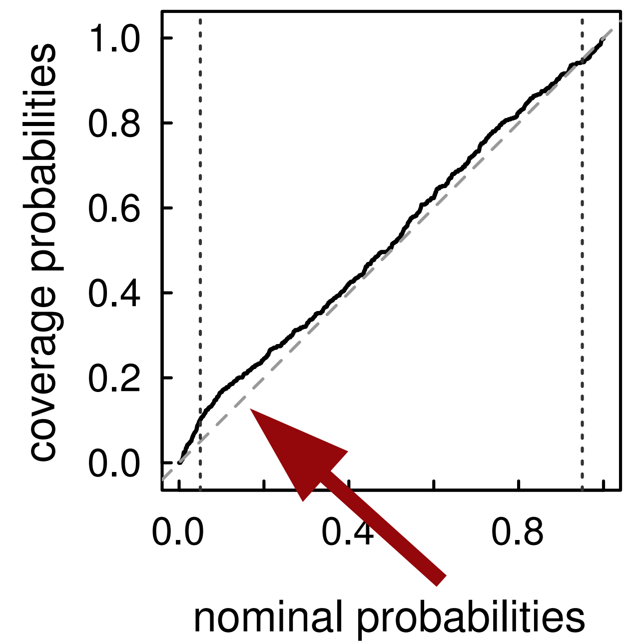
Evaluation of prediction intervals

coverage 90 %-intervals

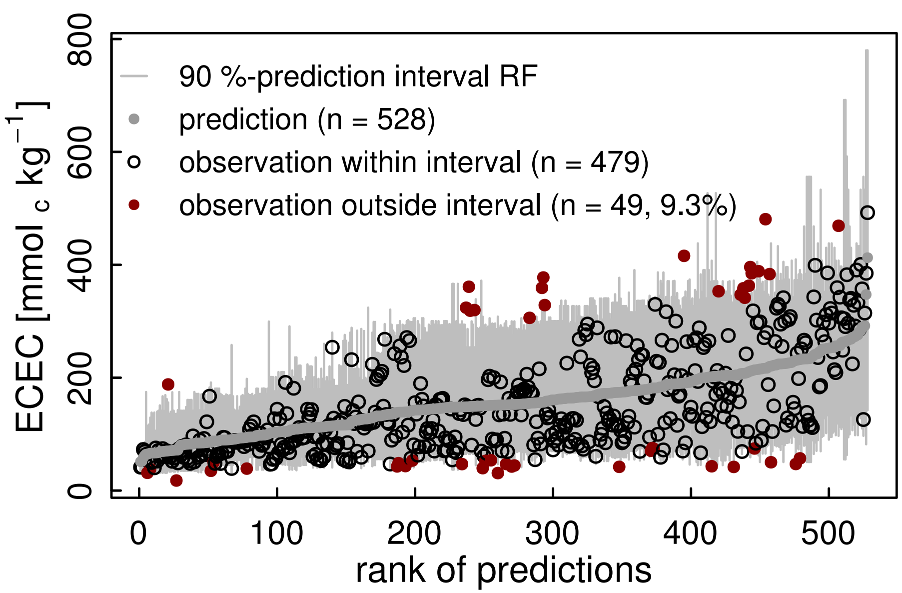
coverage one-sided intervals

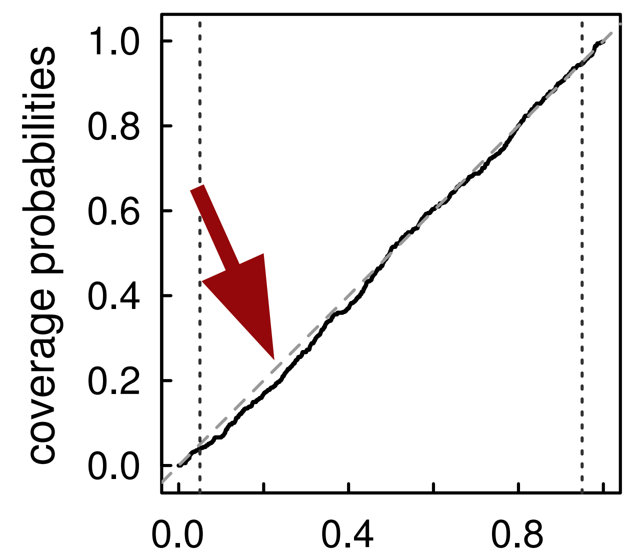
Model-based bootstrap with GAM (non-linear regression)

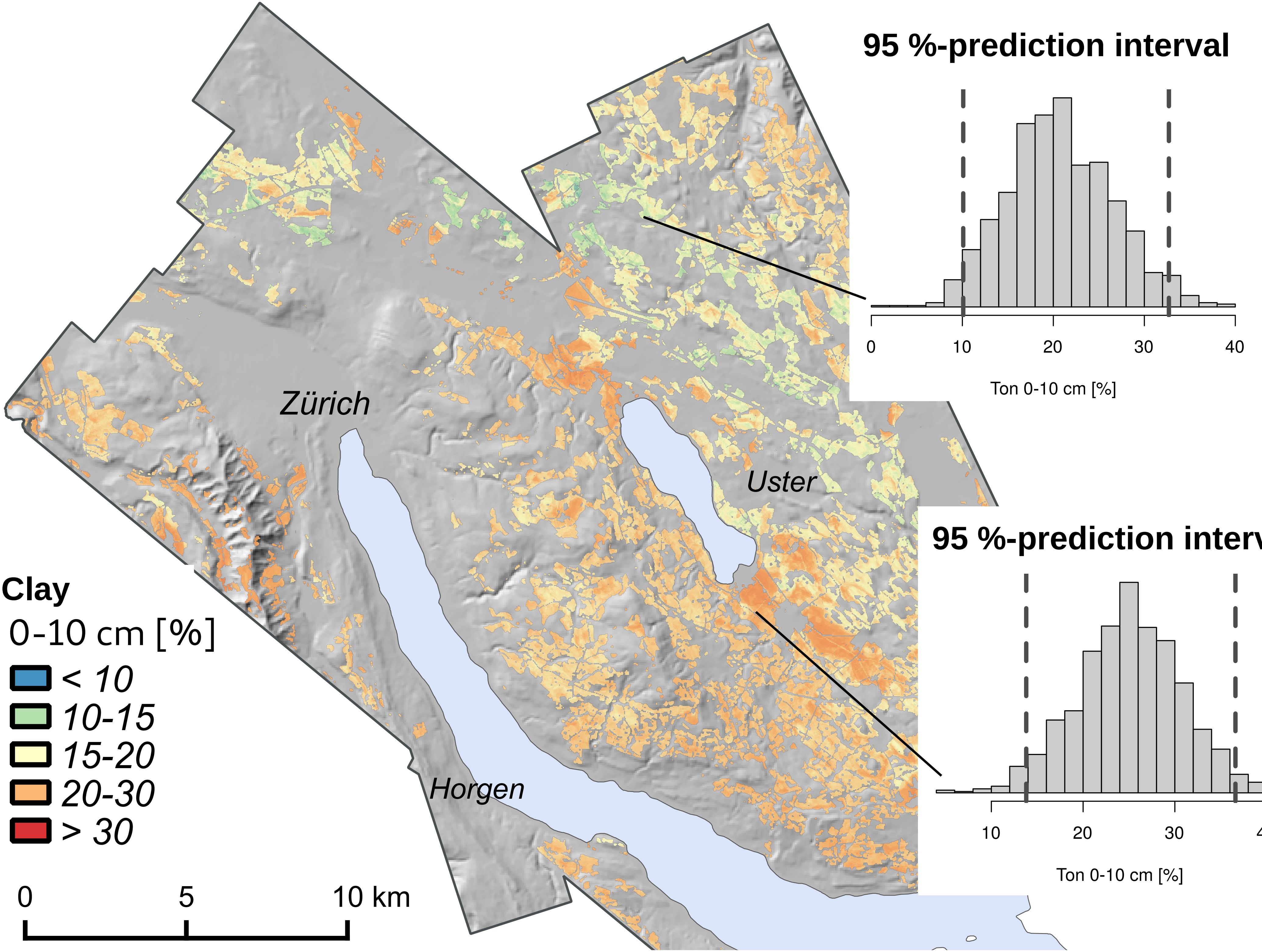




quantile regression forest

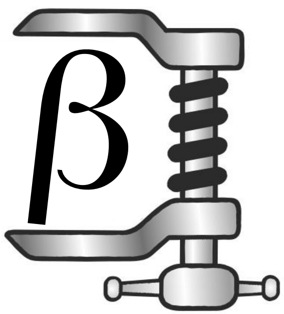


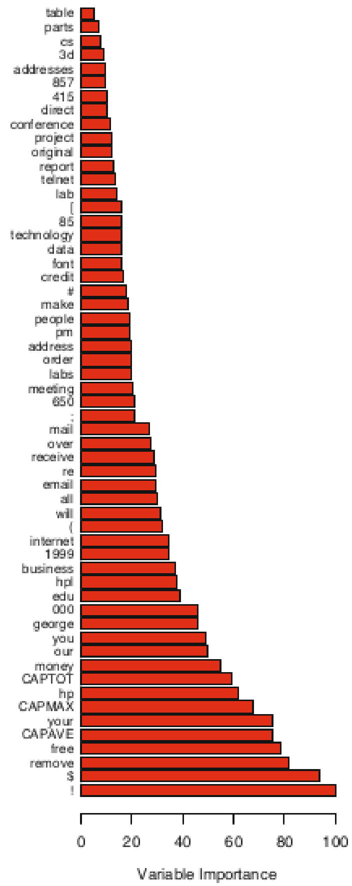


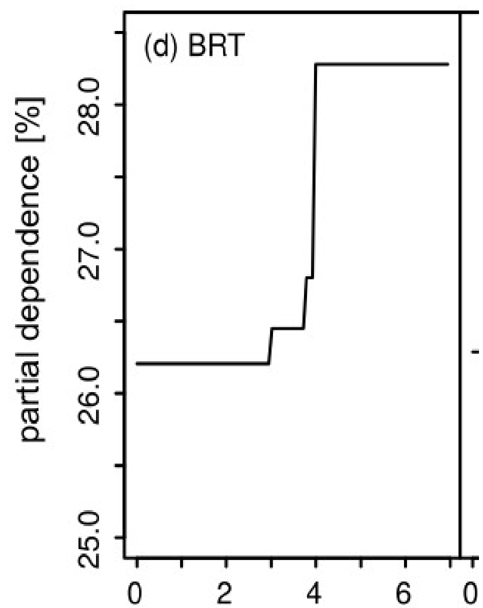


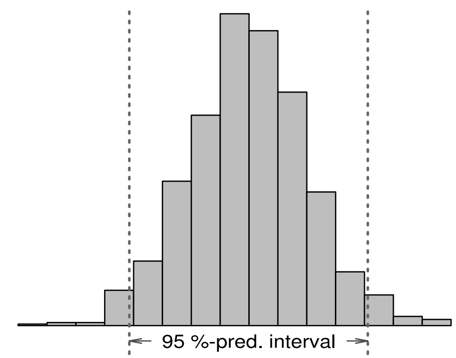
95 %-prediction interval
0
10
20
30
40
Ton 0-10 cm [%]
Zürich
Uster
Horgen
95 %-prediction interv
10
20
30
Ton 0-10 cm [%]
Clay
0-10 cm [%]
< 10
10-15
15-20
20-30
> 30
0
5
10 km

Summary of lecture









My personal tips for your applied ML modelling career:

- **Do not believe there is the ONE solution** (e.g. one model that never fails.). So make sure you understand advantages and disadvantages for your application.
- **Do not neglect classical statistics.** Without understanding linear models you will never master machine learning!
- If a method is hard to understand to you, **please use a simpler one**, that you feel secure with! Your credibility and credibility of your data product is at stake.
- **Do not neglect domain knowledge**. Most likely consulting an expert of your field might improve your model more than the 100redst tuning of the latest fancy method, e.g. by inlcuding a neglected covariate!

Additional literature ...

Davison & Hinkley 1997, on bootstrap methods, a bit technical though.

Davidson, A. C. and Hinkley, D. V.: Bootstrap Methods and Their Applications, Cambridge University Press, Cambridge, doi:10.1017/cbo9780511802843, 1997.

Tutz, 2012, very good book on categorical responses, mostly parametric methods, some ML described, comes with many examples and a R package:

Tutz, G.: Regression for Categorical Data, Cambridge University Press, doi:10.1017/cbo9780511842061, 2012.

Wilks 2011, Useful book for validation measures including for uncertainty, see chapter 8 and R package “verification”:

Wilks, D. S.: Statistical Methods in the Atmospheric Sciences, Academic Press, 3 edn., 2011.

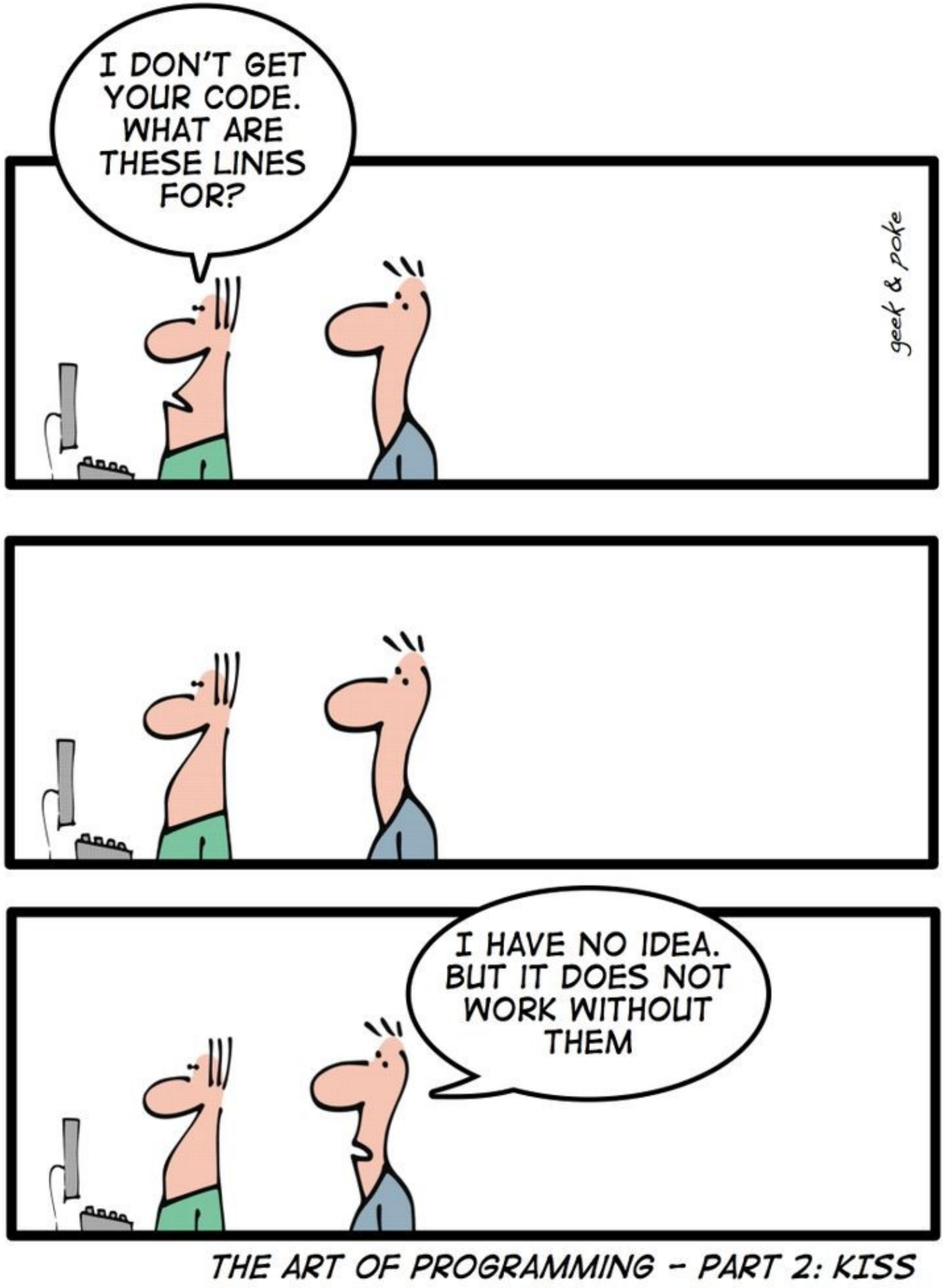
Practical training

You will learn:

model selection

model interpretation

and much more!



http://geekandpoke.typepad.com/geekandpoke/2009/07/the-art-of-programming-part-2.html