ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

WSL

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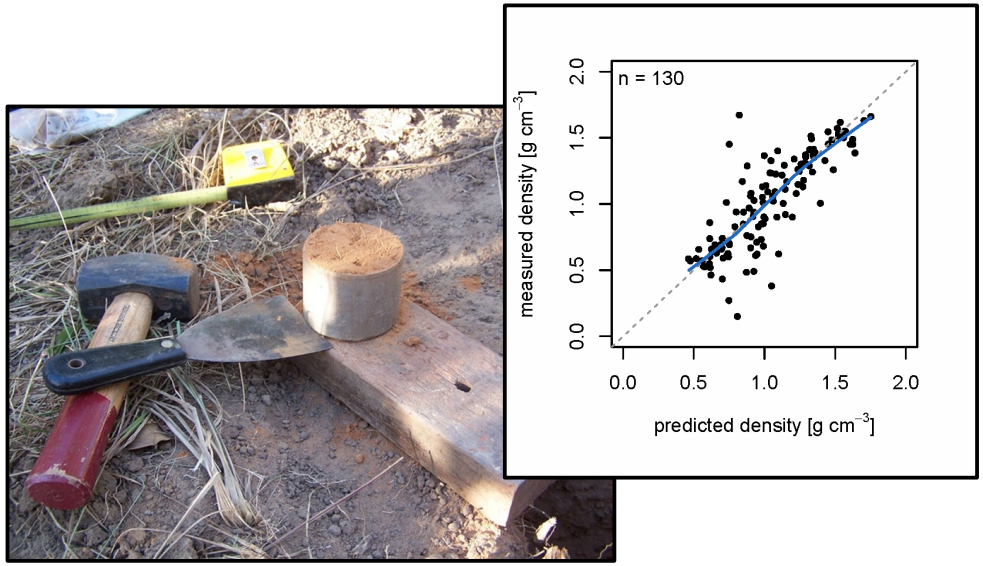
Institute of Terrestrial Ecosystems

Predicting density of Swiss forest soils by component wise gradient boosting



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Soil density: Why?

Important soil parameter e. g. for

- calculations of stocks (nutrients, soil organic carbon [SOC])
- water holding capacity / soil porosity
- evaluation of soil compaction

My presentation

- how is it measured..
- what if no measurements available..
- why did we work on it right now..
- what data and method we used..
- how is this method working..
- what we found..

Soil density measurements

Method

- sampling of volumetric cores in soil pits
- drying at 105° C
- for density of fine soil fraction (< 2mm): sieving

Problems

- large work input (cost)
- large variability (compaction at sampling)
- bias (cores preferentially taken at spots with less gravel)

→ repeated measurements per horizon

Picture sources: www.geologie-service.de/labor.htm, http://prometheuswiki.publish.csiro.au

Pedotransfer rules / functions

- soil density is correlated with other soil properties that are easier to measure
- attempts have been made to give general transfer function
- parameters mostly used:
  soil organic carbon, organic matter, grain size (clay etc.)

Alexander (1980)	$\rho_b = 1.660 - 0.308\ (OC)^{1/2}$
Manrique and Jones (1991)	$\rho_b = 1.660 - 0.318\ (OC)^{1/2}$
Tamminen and Starr (1994)	$\rho_b = 1.565 - 0.2298\ (LOI)^{1/2}$
Adams (1973)	$\rho_b = 100/\{(LOI/0.311) + [(1$
Rawls and Brakensiek (1985)	$\rho_b = 100/\{(LOI/0.224) + [(1$
Honeysett and Ratkowsky (1989)	$\rho_b = (0.548 + 0.0588\ LOI)^{-}$
Federer (1983)	$\ln(\rho_b) = -2.31 - 1.079\ \ln(O$
Huntington (1989)	$\ln(\rho_b) = -2.39 - 1.316\ \ln(O$
Kaur et al. (2002)	$\ln(\rho_b) = 0.313 - 0.191\ OC$

Excerpt of overview by De Vos (2005)

Drawbacks

- transfer to other study regions is limited!
- negative bias: underestimation of density (de Vos, 2005)
- recalibration necessary

Project at WSL:
Forests soils and water balance in a changing climate

Background: Modeling of water retention curve for Swiss forests soils

Required soil parameters: soil texture, soil density, organic matter

Available data

- Measured densities at only 210 forest sites
- Other soil properties available from ~ 3'000 sites

Objectives

- develop density pedotransfer function for Swiss forest soil horizons
- evaluation of its performance

soil data (1/3) – what was measured?

- Density **measurements**: ~ 839 horizon (210 profile sites)
- 3 repeated measurements → median used
- For same horizons **partially** data on:
  - slope, soil depth, sample depth, horizon thickness
  - field estimate of organic matter
    of soil color (hue, value, chroma)
    of gravel content
    of density (5 classes)
  - share of sand, silt, clay fraction
  - pH, SOC content
  - cation exchange capacity, base saturation, total nitrogen content
  - wetness characteristics (9 categories),
    soil depth limitation by rock or ground water

soil data (2/3) – missing values in covariates

problem: data set of covariates (soil properties) incomplete in calibration set, but also in prediction data.

- prediction set incomplete: *soil color*

1) imputation (e.g. with „missforest" using Random Forest)

- precondition: subset with NA are not biased
- check of descriptive statistics → imputation not possible here

2) eliminate missing values

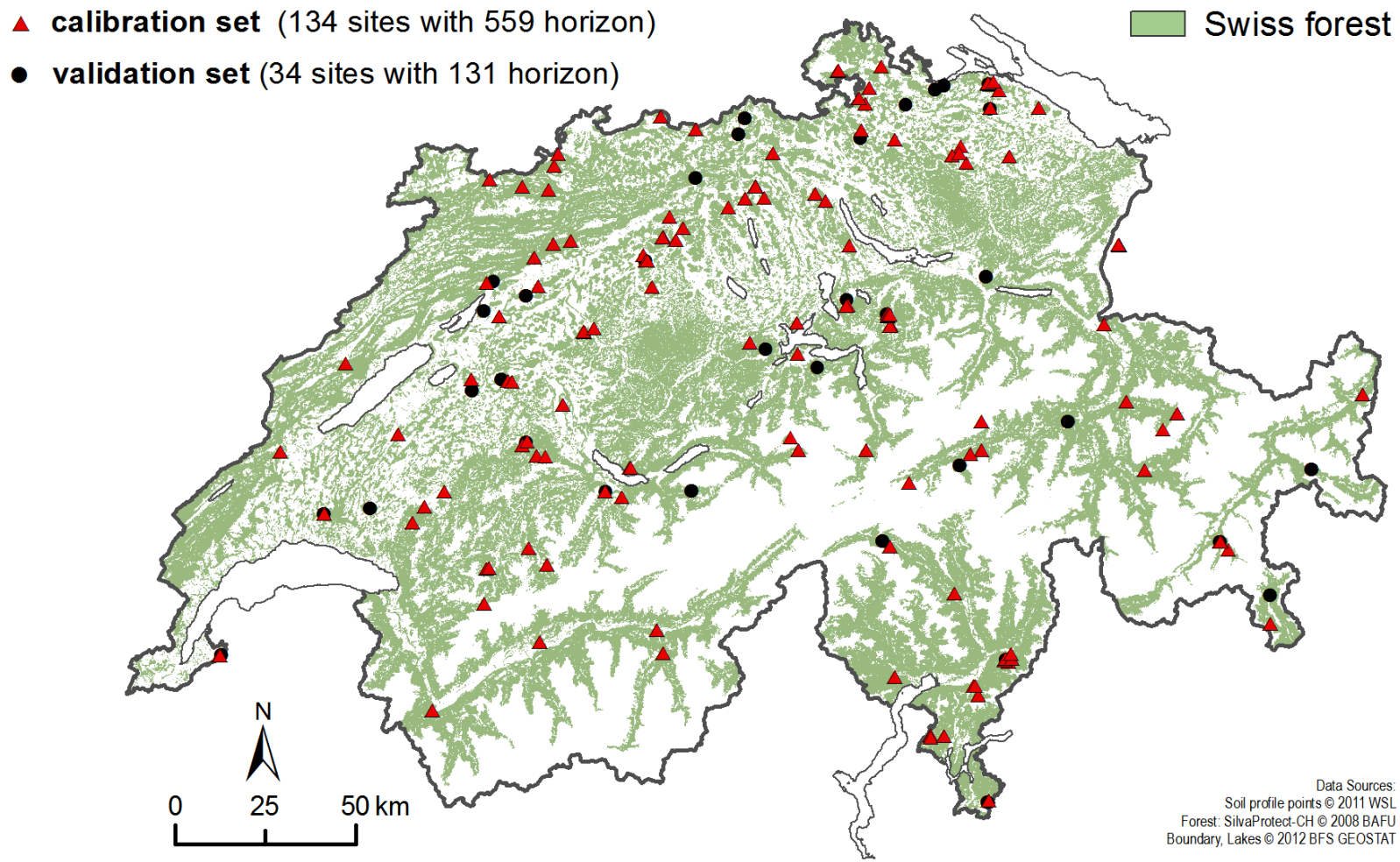
a) omit soil horizon with NA

- *SOC (127 horizons)*

b) omit covariate with large amount of NA

- *total nitrogen, cation exchange capacity, basic saturation*

soil data (3/3) – profile location



Method (1/3) – componentwise gradient boosting

- „weak" learner algorithm
  (small step size ν)
- base-learners, e.g.
  - linear
  - smooth nonlinear
  - trees
- base-learners summed up for prediction

$$\underbrace{Y(s)}_{\text{measurement at point } \boldsymbol{s}} = \underbrace{\sum_j f(x(s))_j}_{\text{Sum of components based on covariates and coordinates}} + \underbrace{\epsilon(s)}_{\text{independent error}}$$

Initialize parameters ($\beta = 0$)

→ 1. Compute residuals (negative gradient)

→ 2. Fit base-learners and select best fitting

→ 3. Update parameters stepwise as sum of previously fitted estimates of the base-learners $f^m = f^{m-1} + \nu u^m$

→ Find optimal number of iterations

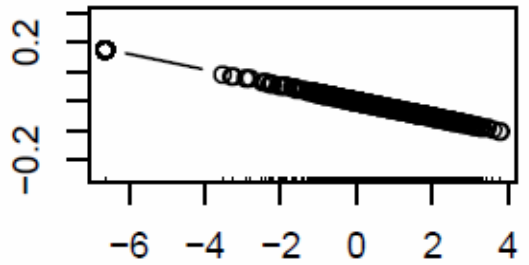
Method (2/3) – advantages

- non-linearity
- smooth spatial surface
- exclusion of non-relevant covariates
- good predictive power expected
- robust loss functions
- interpretability
  (depending on base-learners)

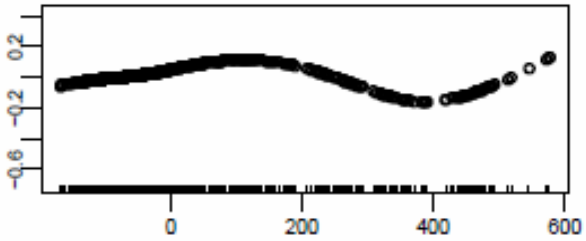
overfitting?

partial residual plots

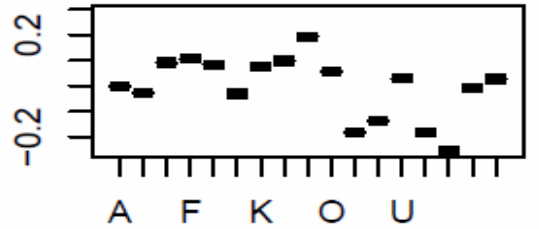
linear base-learner



penalized spline base-learner



linear base-learner (categories)



Method (3/3) – model building and selection

Model $$Y = \underbrace{X\beta}_{\text{linear}} + \underbrace{f(x_1)}_{\text{smooth}} + \underbrace{f(x_1 * x_2)}_{\text{interaction}} + \ldots + \epsilon$$

Model building

A. transformation of response and covariates

1. Box-Cox transformation / log / sqrt

B. selection of relevant covariates

2. selection of **linear** covariates by 10fold cross-validation

3. **merge** categories of selected covariates with partial residual plots

➡

4. fit boosting with **smooth** covariates on **residuals**

5. select final model with residual plots and cross-validation

Resulting Model

resulting model (1/2) – linear parameters

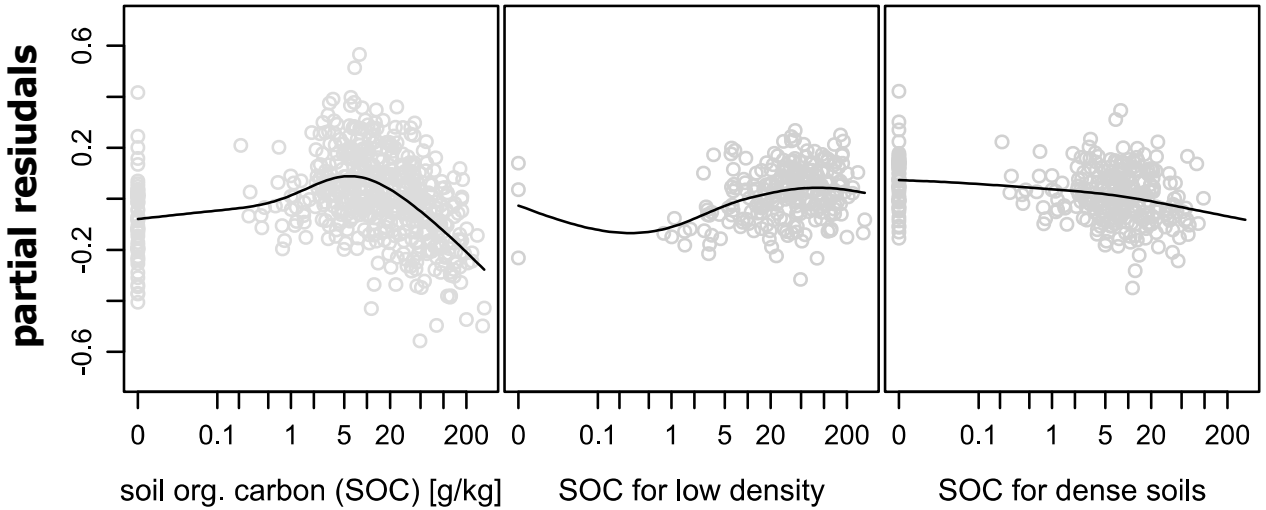
linear parameters in best-fit model:

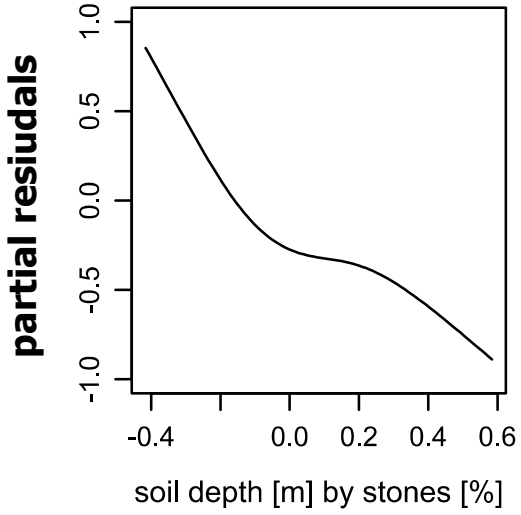
- ↑ sample depth (sqrt)
- ↓ slope angle (sqrt)
- ↑ field estimate of density (3 classes)
- ↓↑ 8 aggregated soil map units (1:200'000)

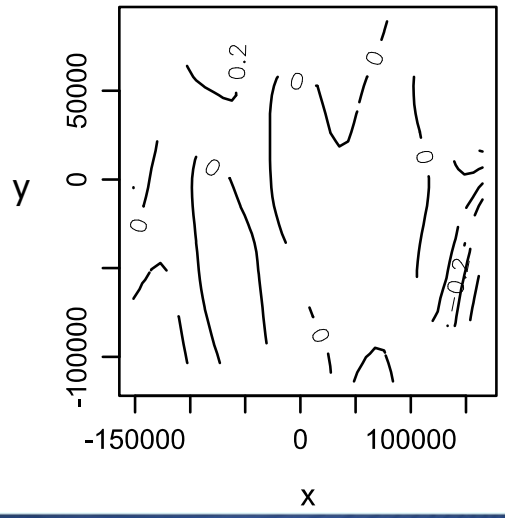
linear interactions in best-fit model:

- ↓↑ profile depth for 5 soil map units
- ↓↑ share of silt and clay / soil organic carbon (SOC) for unlimited, ground water or rock limited soils

resulting model (2/2) – smooth elements



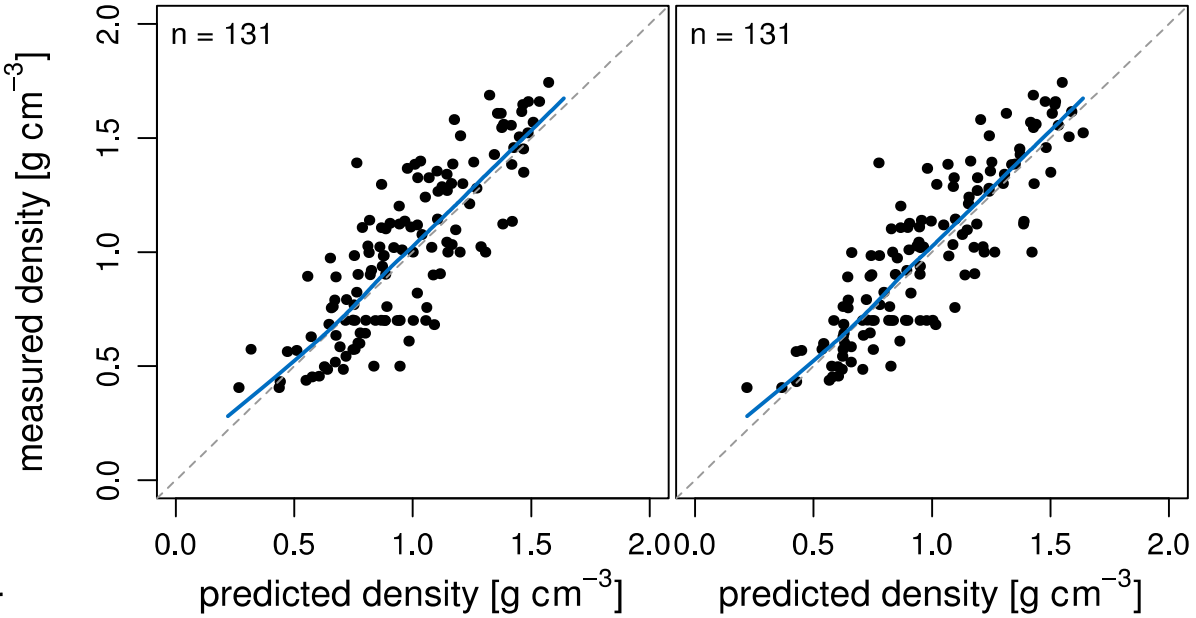




Model Performance

Validation with measurements of 131 horizon not used for calibration.

	Linear	Linear + Smooth
RMSE / MADE *	0.205 / 0.235	0.178 / 0.188
R^2 (robust)	0.669	0.771



* root mean squared error,
median absolute deviation error

Summary / Conclusion

- **expanded pedotransfer function** with 8 input covariates and spatial position
- model improvement by including **non-linear terms** with boosting algorithm
- **succesfull model selection** without overfitting
- **satisfactory model performance** (robust $R^2 = 0.77$ with indepenent validation set)

Outlook

- Investigate in final fit with robust methods
- Investigate in predictive distribution to compute standard errors to the predictions