Model Choice and Variable Selection in Geoadditive Regression Models

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joint work with

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Geoadditive Regression: Forest Health Example

- Aim of the study: Identify factors influencing the health status of trees.

- Database: Yearly visual forest health inventories carried out from 1983 to 2004 in a northern Bavarian forest district.

- 83 observation plots of beeches within a 15 km times 10 km area.

- Response: binary defoliation indicator $y_{it}$ of plot $i$ in year $t$ ($1 = \text{defoliation higher than 25\%}$).

- Spatially structured longitudinal data.
- **Covariates:**

  **Continuous:**
  - average age of trees at the observation plot
  - elevation above sea level in meters
  - inclination of slope in percent
  - depth of soil layer in centimeters
  - pH-value in 0 – 2cm depth
  - density of forest canopy in percent

  **Categorical**
  - thickness of humus layer in 5 ordered categories
  - level of soil moisture
  - base saturation in 4 ordered categories

  **Binary**
  - type of stand
  - application of fertilisation
• Possible model:

\[ P(y_{it} = 1) = \frac{\exp(\eta_{it})}{1 + \exp(\eta_{it})} \]

where \( \eta_{it} \) is a geoadditive predictor of the form

\[ \eta_{it} = f_1(\text{age}_{it}, t) + \text{interaction between age and calendar time.} \]

\[ f_2(\text{canopy}_{it}) + \text{smooth effects of the canopy density and} \]

\[ f_3(\text{soil}_{it}) + \text{the depth of the soil layer.} \]

\[ f_{\text{spat}}(s_{ix}, s_{iy}) + \text{structured and} \]

\[ b_i + \text{unstructured spatial random effects.} \]

\[ x'_{it}/\beta \text{ parametric effects of type of stand, fertilisation,} \]

\[ \text{thickness of humus layer, level of soil moisture} \]

\[ \text{and base saturation.} \]
Questions:

- How do we estimate the model? ⇒ Inference.
- How do we come up with the model specification? ⇒ Model choice and variable selection.

⇒ Componentwise boosting for geoadditive regression models.
Componentwise base-learning procedures for geoadditive regression models can be derived from univariate Gaussian smoothing approaches such as

\[ y = g(x) + \varepsilon \] smooth nonparametric effect
\[ y = g(x_1, x_2) + \varepsilon \] smooth surface / spatial effect
\[ y = x_1 g(x_2) + \varepsilon \] varying coefficients

where \( \varepsilon \sim N(0, \sigma^2 I) \).

All base-learners will be given by penalised least squares (PLS) fits

\[ \hat{y} = X(X'X + \lambda K)^{-1} X'y \]

characterised by the hat matrix

\[ S_\lambda = X(X'X + \lambda K)^{-1} X'. \]
• Recall univariate penalised spline smoothing: Approximate \( g(x) \) by a linear combination of B-spline basis functions, i.e.

\[
g(x) = \sum_j \beta_j B_j(x)
\]

and define a difference penalty

\[
\text{pen}(\beta) = \lambda \sum_j (\beta_j - \beta_{j-1})^2 \quad \text{or} \quad \text{pen}(\beta) = \lambda \sum_j (\beta_j - 2\beta_{j-1} + \beta_{j-2})^2.
\]

to ensure smoothness.

• Model and penalty in matrix notation:

\[
y = X\beta + \varepsilon \quad \text{and} \quad \text{pen}(\beta) = \lambda \beta'K\beta.
\]

• Penalised least squares estimate and fit:

\[
\hat{\beta} = (X'X + \lambda K)^{-1}X'y \quad \hat{y} = X(X'X + \lambda K)^{-1}X'y.
\]
• PLS base-learner for interaction surfaces and spatial effects \( f(x_1, x_2) \):

\[
B_{jk}(x_1, x_2) = B_j(x_1)B_k(x_2).
\]

• Define bivariate Tensor product basis functions

\[
\text{pen}(\beta) = \lambda \beta' \left( I \otimes K_1 + K_2 \otimes I \right) \beta.
\]
• PLS base-learner for varying coefficient terms

\[ y = x_1 g(x_2) + \varepsilon \]

Representing \( g(x_2) \) as a penalised spline yields \( y = X \beta + \varepsilon \), where

\[ X = \text{diag}(x_{11}, \ldots, x_{n1}) X^* \]

and \( X^* \) is the design matrix corresponding to \( g(x_2) \).

• PLS base-learners can also be defined for
  
  – Random intercepts and random slopes,
  
  – Space-varying effects.
Complexity Adjustment

- The flexibility of penalised least squares base-learners depends on the choice of the smoothing parameter.

- Typical strategy: fix the smoothing parameter at a large pre-specified value.

- Difficult when comparing fixed effects, nonparametric effects and spatial effects.

  ⇒ More flexible base-learners will be preferred in the boosting iterations leading to potential selection and estimation bias.

- We need an intuitive measure of complexity.

- Effective degrees of freedom of a penalised least-squares base-learner:

  \[
  \text{df}(\lambda) = \text{trace}(X(X'X + \lambda \mathbf{K})^{-1}X').
  \]
• Choose the smoothing parameters for the base-learners such that

\[ df(\lambda) = 1. \]

• Can not be achieved for most base-learners since

\[ \lim_{\lambda \to \infty} df(\lambda) \geq 1. \]

• For example, a polynomial of order \( k - 1 \) remains unpenalised for penalised splines with \( k \)-th order difference penalty.

• A reparameterisation has to be applied, leading for example to

\[ f(x) = \beta_0 + \beta_1 x + \ldots + \beta_{k-1} x^{k-1} + f_{\text{centered}}(x). \]

• Assign separate base-learners to the parametric components and a one degree of freedom PLS base-learner to the centered effect.
Boosting Geoadditive Regression Models

- Generic representation of geoadditive models:

\[ \eta(\cdot) = \beta_0 + \sum_{j=1}^{r} f_j(\cdot) \]

where the functions \( f_j(\cdot) \) represent the candidate functions of the predictor.

- Each candidate function is associated with a PLS base-learner.

- Early stopping of the boosting algorithm implements variables selection.

- Defining concurring base-learners implements model choice (for example linear vs. nonlinear modelling).

- The number of boosting iterations can be determined based on AIC reduction or cross-validation.
Habitat Suitability Analyses

- Identify factors influencing habitat suitability for breeding bird communities collected in seven structural guilds (SG).

- Variable of interest: Counts of subjects from a specific structural guild collected at 258 observation plots in a Northern Bavarian forest district.

- Research questions:
  a) Which covariates influence habitat suitability (31 covariates in total)? Does spatial correlation have an impact on variable selection?
  b) Are there nonlinear effects of some of the covariates?
  c) Are effects varying spatially?

- All questions can be addressed with the boosting approach (but we focus on a)).
## Selection frequencies in a spatial Poisson-GLM:

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- A similar picture is obtained from considering the estimated regression coefficients.
• Spatial effects for high and low degrees of freedom:

![5 df spatial effect](image1)

![1 df spatial effect](image2)

• Spatial correlation has non-negligible influence on variable selection.

• Making terms comparable in terms of complexity is essential to obtain valid results.
Summary & Extensions

- Generic boosting algorithm for model choice and variable selection in geoadditive regression models.

- Avoid selection bias by careful parameterisation.

- Implemented in the R-package mboost.

- Future plans:
  - Derive base-learning procedures for other types of spatial effects (regional data, anisotropic spatial effects).
  - Construct spatio-temporal base-learners based on tensor product approaches.

• Find out more:

    http://www.stat.uni-muenchen.de/~kneib