Analysing Spatio-temporal Regression Data: A Case Study in Forest Health

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MATHEMATIK UND
NATURWISSENSCHAFTEN

Göttingen, 4.6.2009

Spatio-Temporal Regression Data

- Regression in a general sense:
  - Linear models and generalised linear models,
  - Multivariate (categorical) generalised linear models,
  - Regression models for duration times (Cox-type models, AFT models).
- Common structure: Model a quantity of interest in terms of categorical and continuous covariates, e.g.

$$\mathbb{E}(y|x) = h(x'\beta) \qquad \text{(GLM)}$$

or

$$\lambda(t|x) = \lambda_0(t)\exp(x'\beta) \qquad \text{(Cox model)}$$

- Spatio-temporal data: Temporal and spatial information as additional covariates.

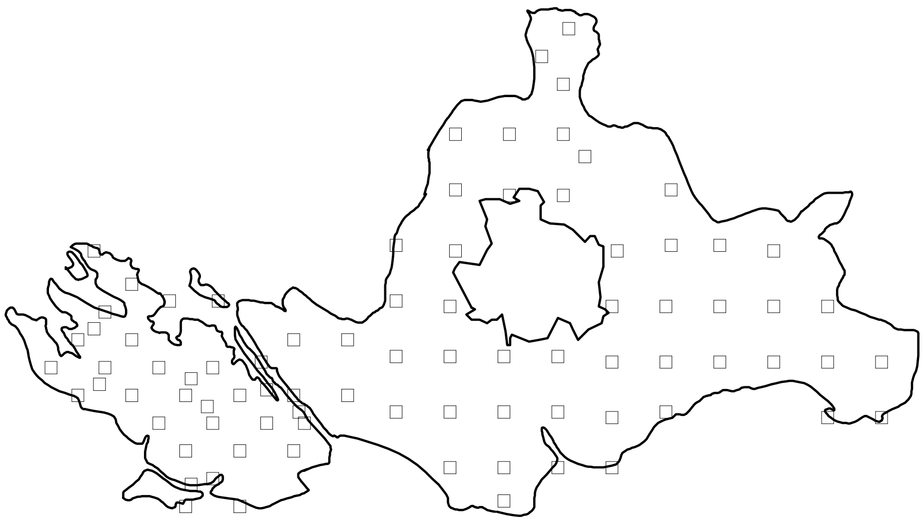
- Spatio-temporal regression models should allow
  - to account for spatial and temporal correlations,
  - for time- and space-varying effects,
  - for non-linear effects of continuous covariates,
  - for flexible interactions,
  - to account for unobserved heterogeneity.

$\Rightarrow$ Geoadditive regression models.

Case Study: Forest Health Data

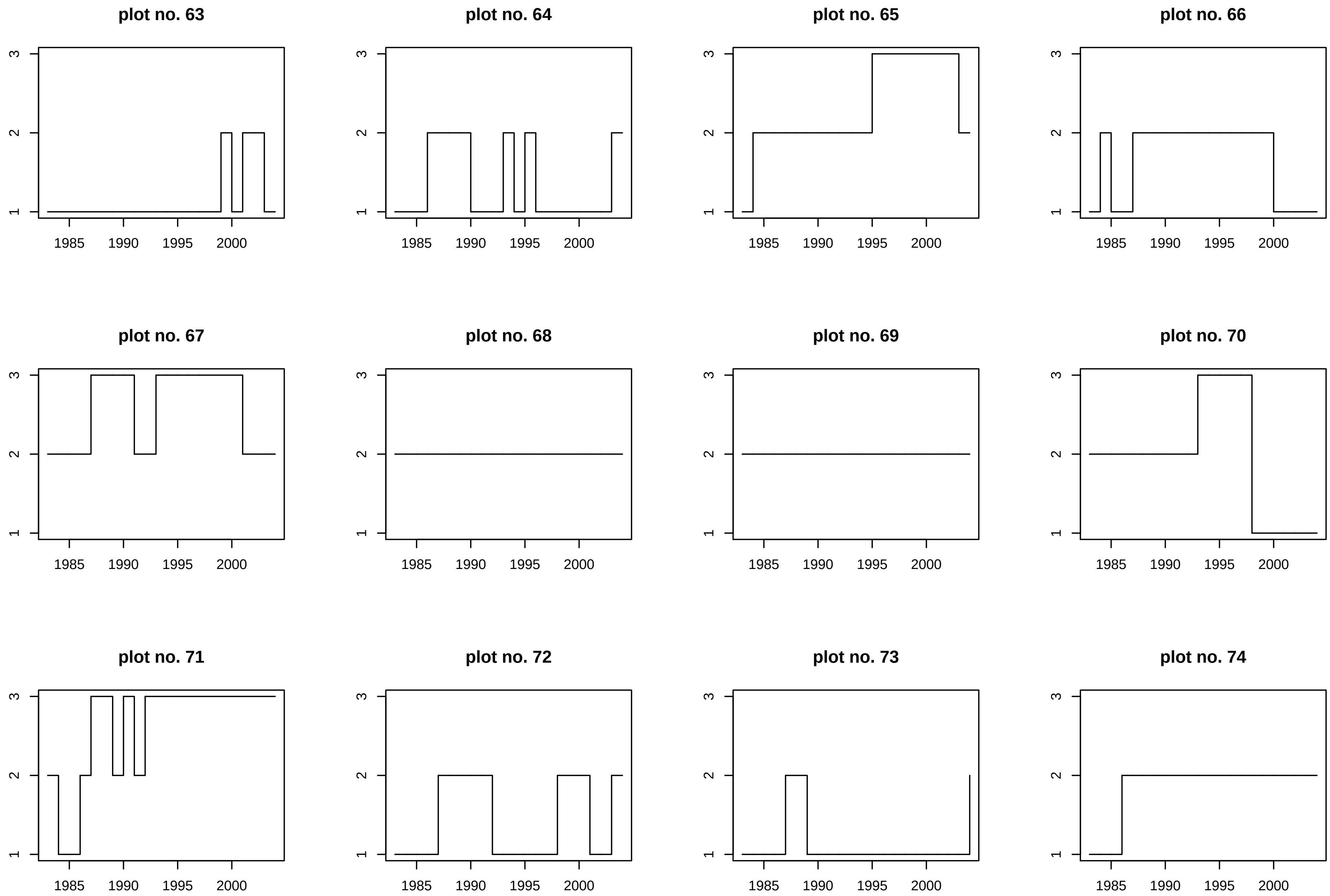
- Aim of the study: Identify factors influencing the health status of trees.
- Database: Yearly visual forest health inventories carried out from 1983 to 2004 in a northern Bavarian forest district.
- 83 observation plots of beeches within a 15 km times 10 km area.
- Response: defoliation degree at plot i in year t, measured in three ordered categories:

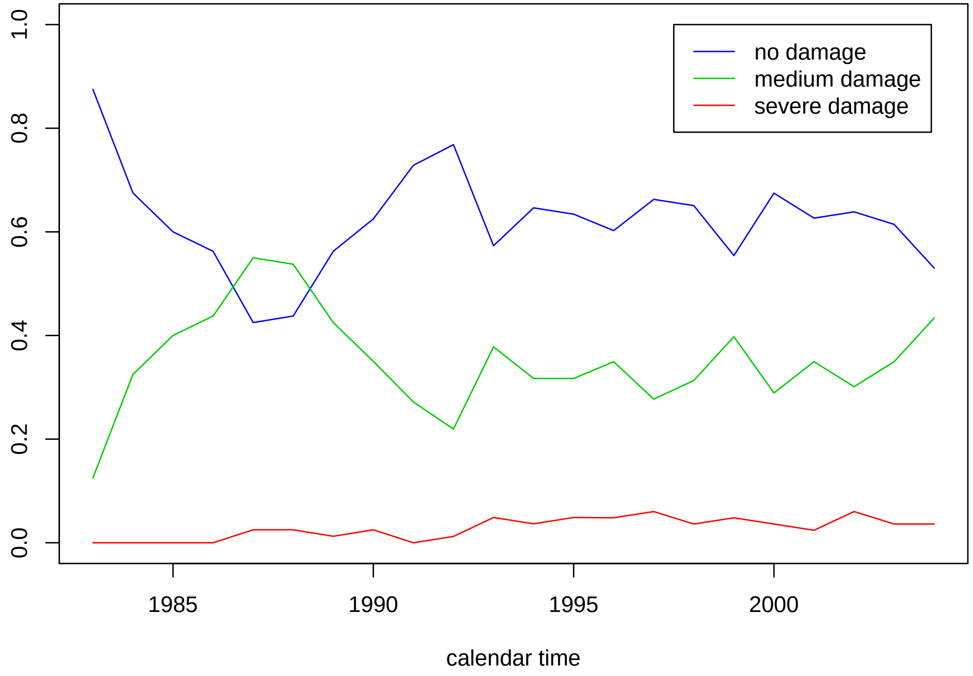
$y_{it} = 1$ no defoliation,
$y_{it} = 2$ defoliation 25% or less,
$y_{it} = 3$ defoliation above 25%.



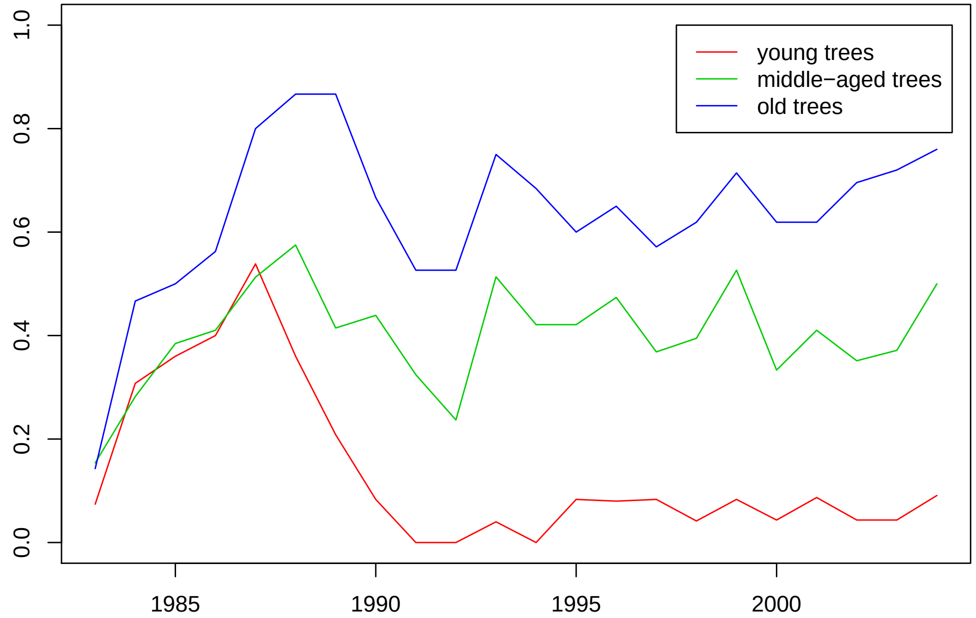
- Covariates:

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

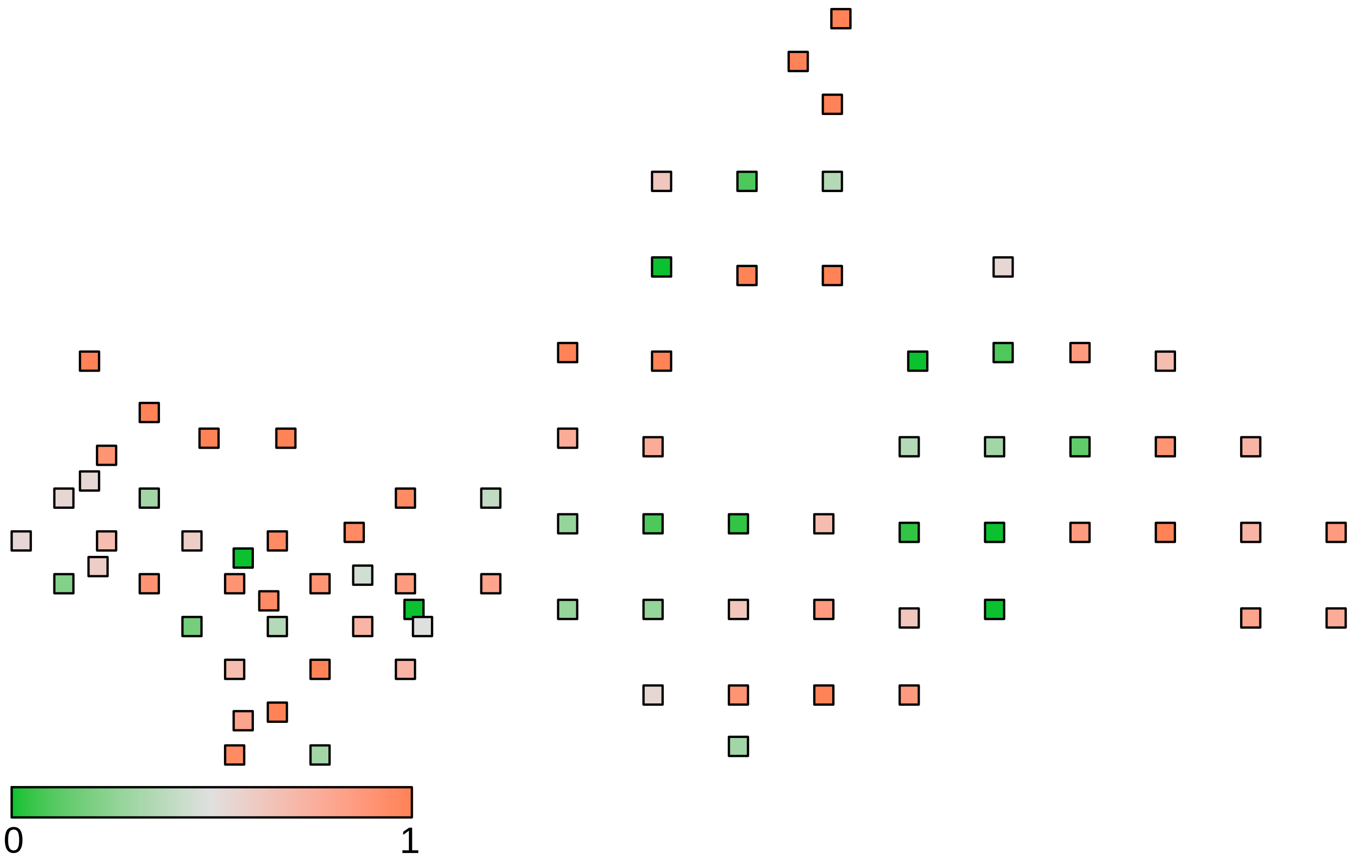

plot no. 63
plot no. 64
plot no. 65
plot no. 66
plot no. 67
plot no. 68
plot no. 69
plot no. 70
plot no. 71
plot no. 72
plot no. 73
plot no. 74



Empirical time trends.



Trends for different ages.



Percentage of time points for which a tree was classified to be damaged.

- We need a regression model that can simultaneously deal with the following issues:
  - A spatially aligned set of time series.

    $\Rightarrow$ Both spatial and temporal correlations have to be considered.
  - Decide whether unobserved heterogeneity is spatially structured or not.
  - Non-linear effects of continuous covariates (e.g. age).
  - A possibly time-varying effect of age (i.e. an interaction between age and calendar time).
  - A categorical response variable.

Regression models for ordinal responses

- Defoliation degree is measured in three ordered categories.
- Derive regression models for ordinal responses based on latent variables:

$$D = x'\beta + \varepsilon.$$

- D can be considered an unobserved, continuous measure of forest damage.
- Link D to the categorical response Y based on ordered thresholds

$$-\infty = \theta^{(0)} < \theta^{(1)} < \theta^{(2)} < \theta^{(3)} = \infty$$

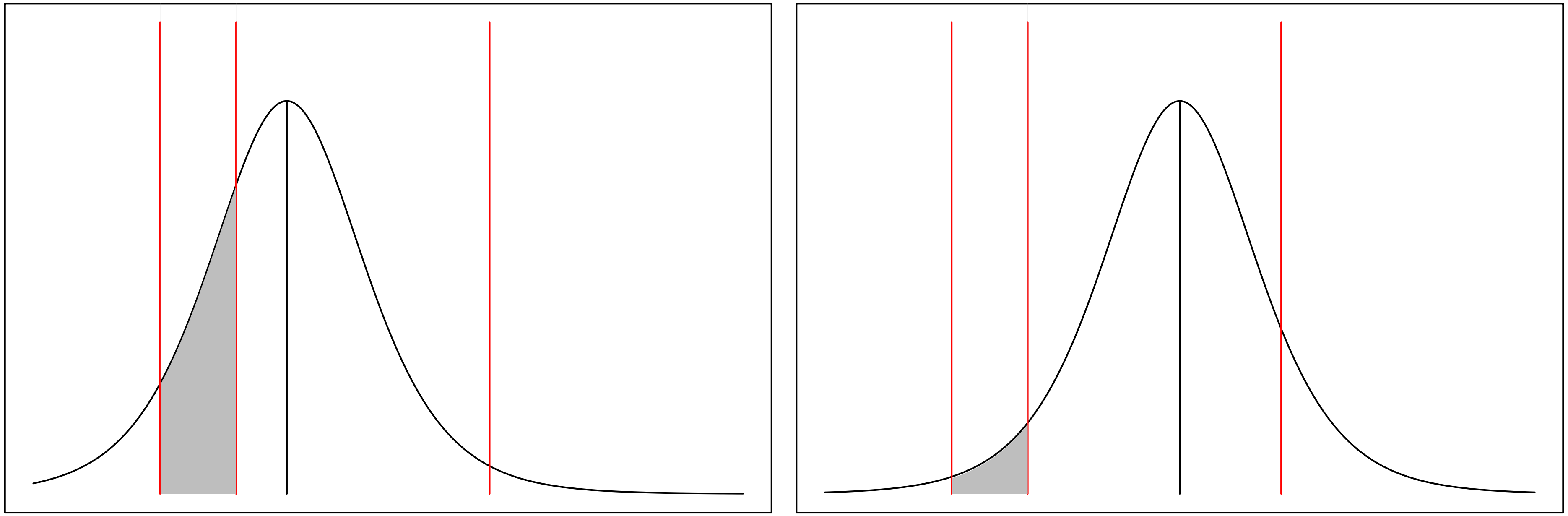
via

$$Y = r \quad \Leftrightarrow \quad \theta^{(r-1)} < D \leq \theta^{(r)}.$$

- Defines cumulative probabilities in terms of the cdf F of the latent error term ε:

$$P(Y \leq r) = P(D \leq \theta^{(r)}) = P(x'\beta + \varepsilon \leq \theta^{(r)}) = F(\theta^{(r)} - x'\beta).$$

- Graphical interpretation:



- The thresholds slice the density $f = F'$.

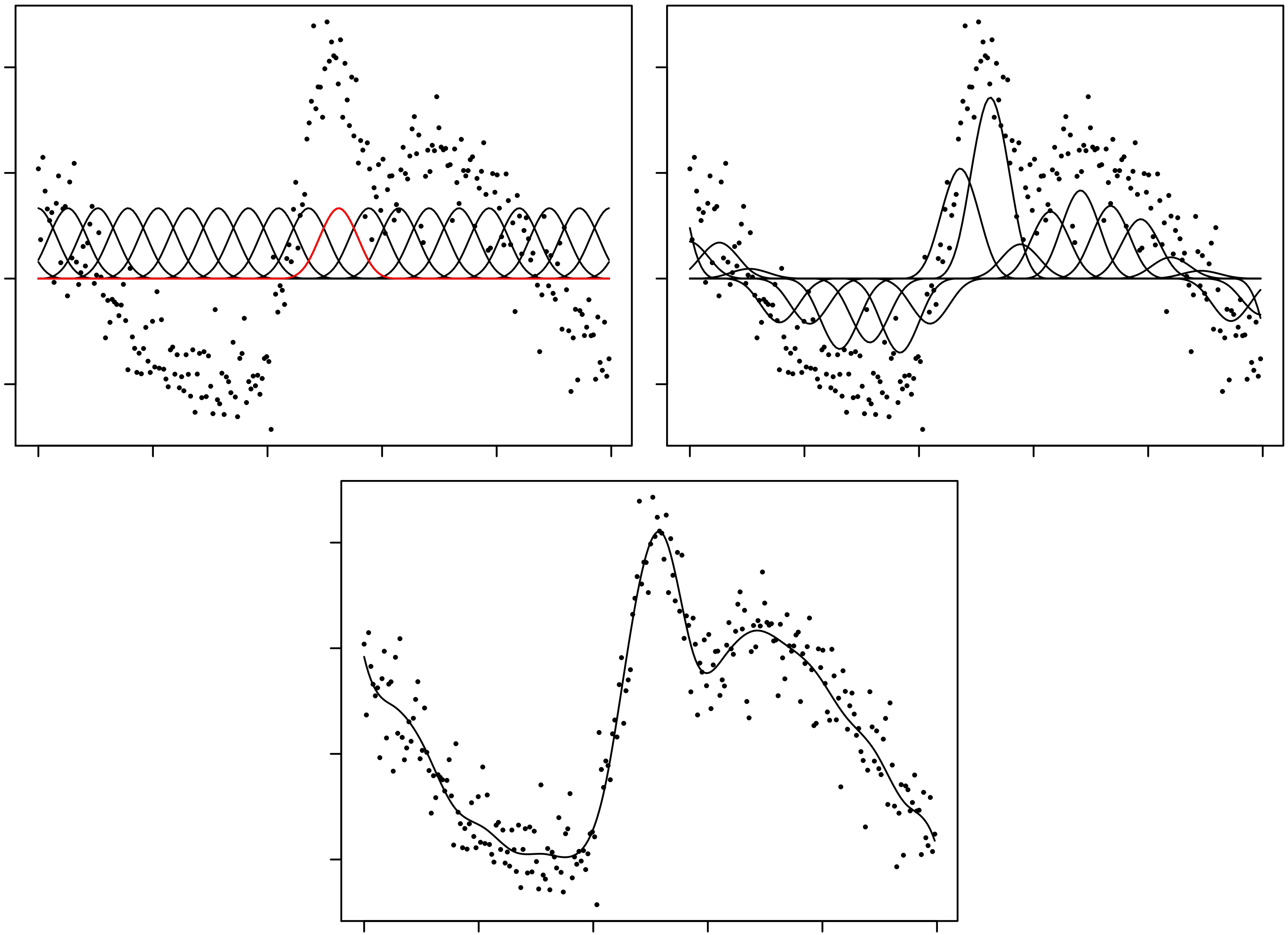
- Suitable model in our application:

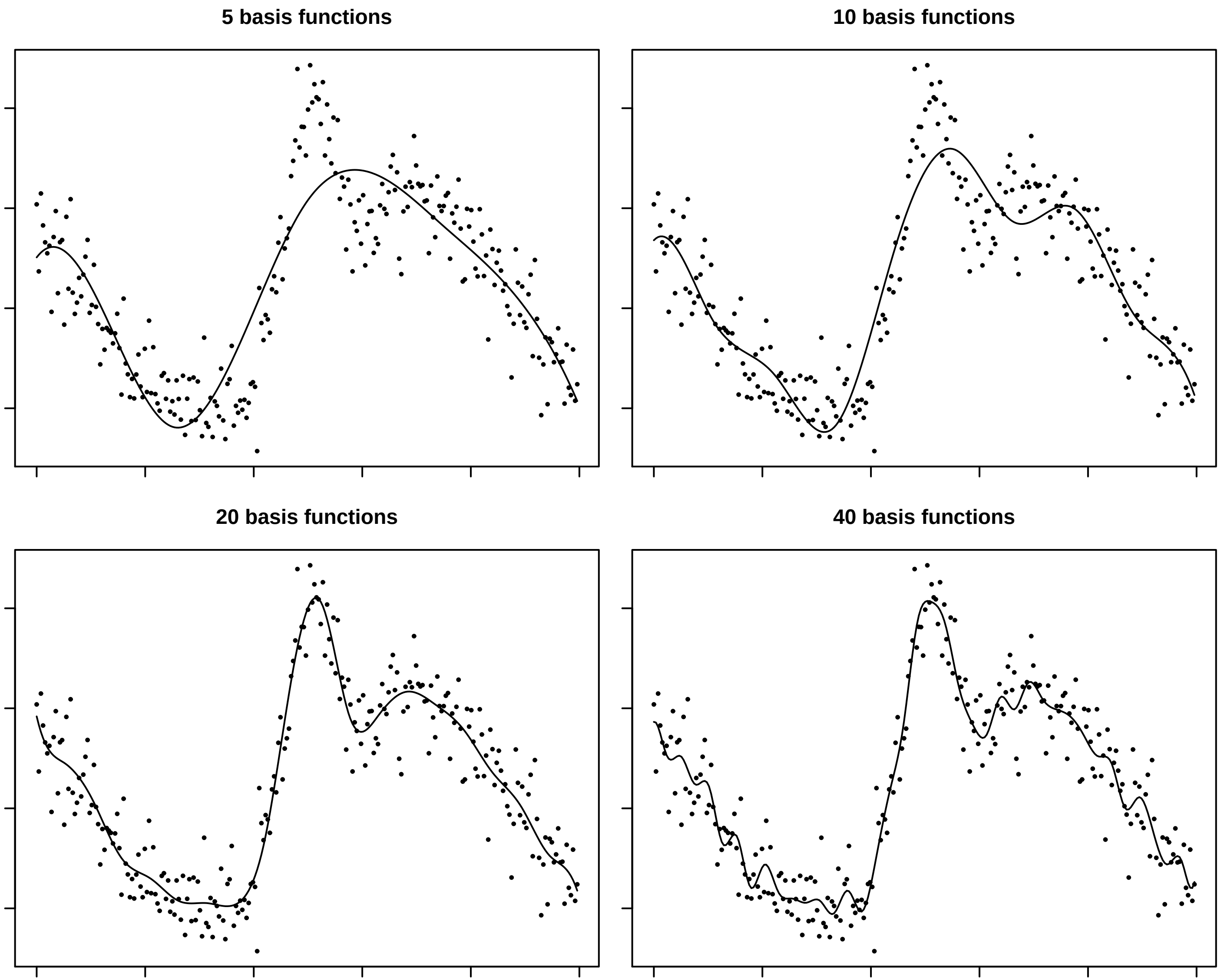
$$
\begin{aligned}
D_{it} \quad = \quad & f_1(age_{it}) && \text{nonlinear effects of age,} \\
& +f_2(inc_i) && \text{inclination of slope, and} \\
& +f_3(can_{it}) && \text{canopy density.} \\
& +f_{time}(t) && \text{nonlinear time trend.} \\
& +f_4(t, age_{it}) && \text{interaction between age and calendar time.} \\
& +f_{spat}(s_i) && \text{structured and} \\
& +b_i && \text{unstructured spatial random effects.} \\
& +x_{it}'\gamma && \text{usual parametric effects.} \\
& +\varepsilon_{it} && \text{error term.}
\end{aligned}
$$

Penalised Splines

- Aim: Model nonparametric trend functions and nonparametric covariate effects.
- Idea: Approximate $f(x)$ (or $f(t)$) by a weighted sum of B-spline basis functions:

$$f(x) = \sum_j \gamma_j B_j(x)$$




5 basis functions
10 basis functions
20 basis functions
40 basis functions

- The number of basis functions has significant impact on the function estimate.
- Employ a large number of basis functions to enable flexibility.
- Penalise differences between parameters of adjacent basis functions to ensure smoothness:

$$\text{pen}(\gamma|\tau^2) = \frac{1}{2\tau^2}\sum_{j=2}^{p}(\gamma_j - \gamma_{j-1})^2 \qquad \text{first order differences}$$

$$\text{pen}(\gamma|\tau^2) = \frac{1}{2\tau^2}\sum_{j=3}^{p}(\gamma_j - 2\gamma_{j-1} + \gamma_{j-2})^2 \qquad \text{second order differences}$$

- A penalty term based on k-th order differences is an approximation to the integrated squared k-th derivative.
- Penalties can be rewritten as quadratic forms

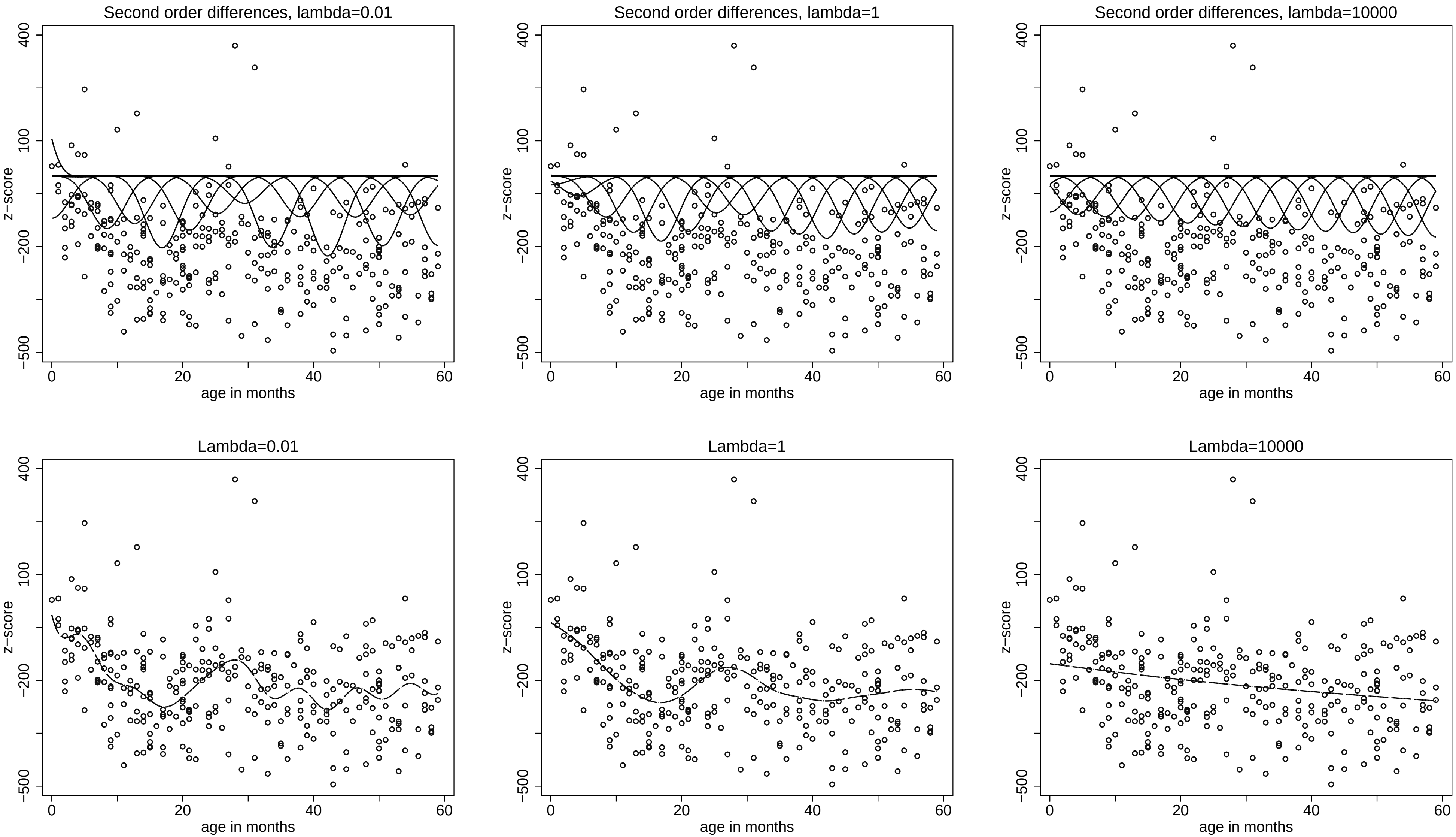
$$\text{pen}(\gamma|\tau^2) = \frac{1}{2\tau^2}\gamma' K \gamma$$

where $K = D'D$ and D is a difference matrix of appropriate order.

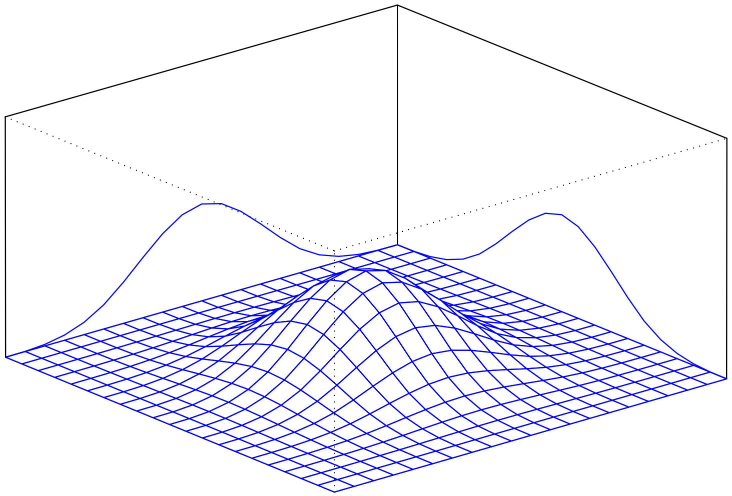
- Penalised maximum likelihood estimation with smoothing parameter τ^2:

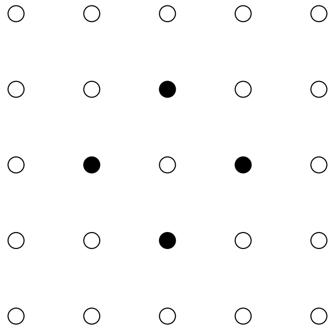
$$l_{\text{pen}}(\gamma) = l(\gamma) - \frac{1}{2\tau^2}\gamma' K \gamma \to \max_{\gamma}$$

- Solution (for given smoothing parameter) can be obtained via penalised Fisher scoring.
- Key question: Automatic selection of the smoothing parameter τ^2.


Second order differences, lambda=0.01
Second order differences, lambda=1
Second order differences, lambda=10000
Lambda=0.01
Lambda=1
Lambda=10000
z−score
400
100
−200
−500
age in months
0
20
40
60

- Extension to bivariate penalised splines:
  - Bivariate basis functions based on tensor product B-splines.
  - Extend penalisation to neighbours on a grid.

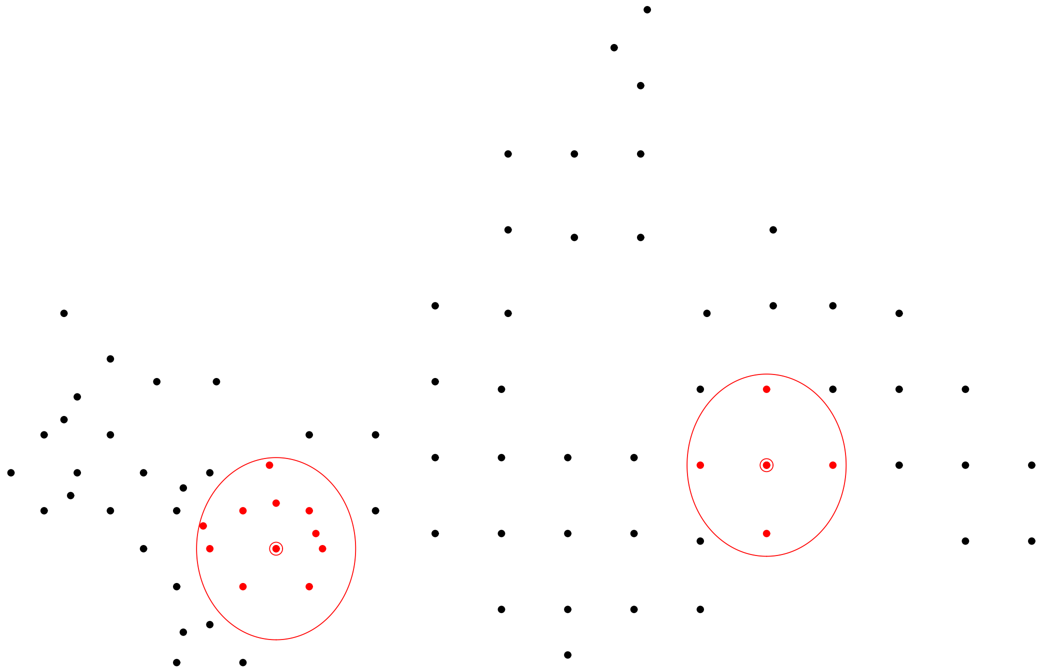




⇒ Modelling of interaction surfaces (and spatial effects).

Spatial Modelling

- Markov random fields: Structured spatial effect.
- Bivariate extension of a first order random walk on the real line.
- Define two observation plots as neighbours if their distance is less than 1.2km.

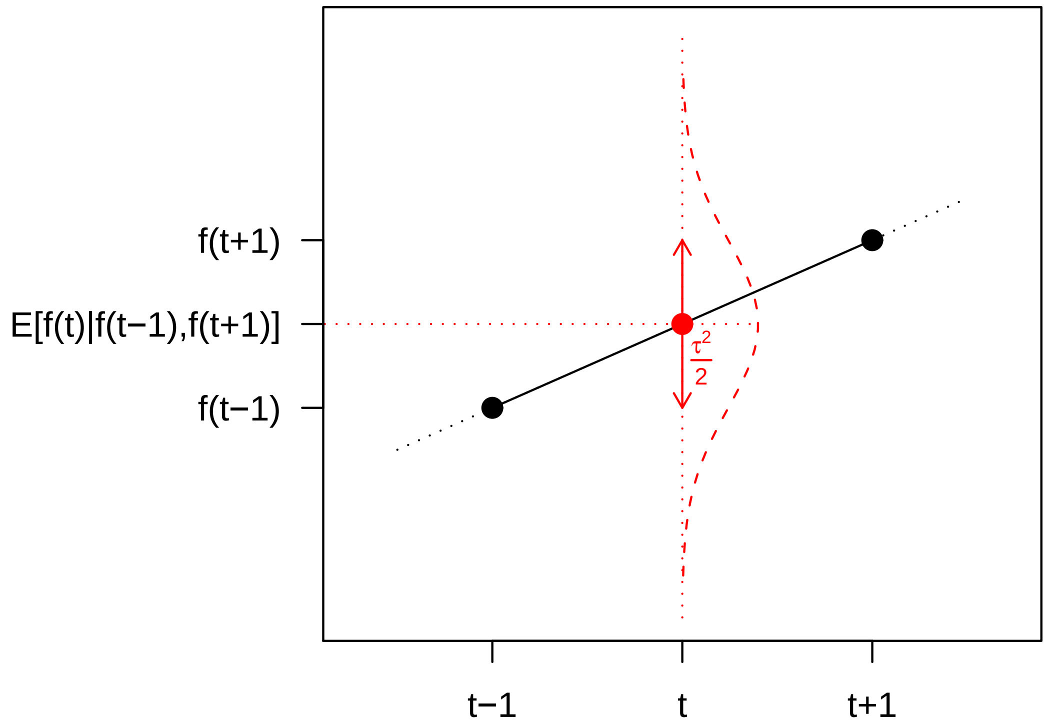


- Assume that the expected value of $\gamma_s = f_{spat}(s)$ is the average of the function evaluations of adjacent sites:

$$\gamma_s | \gamma_r, r \neq s \sim N\left(\frac{1}{N_s}\sum_{r\in\delta_s}\gamma_r, \frac{\tau^2}{N_s}\right)$$

where

δ_s set of neighbors of plot s
N_s no. of such neighbors.



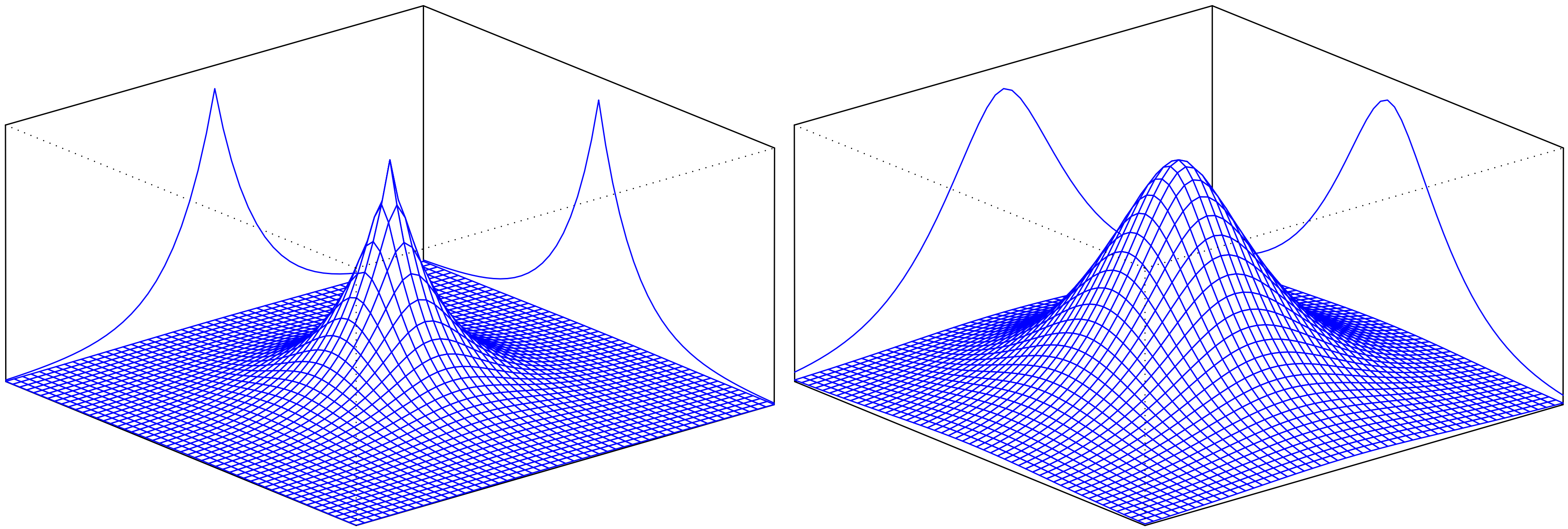
- Equivalent formulation in terms of a difference penalty:

$$\text{pen}(\gamma|\tau^2) = \frac{1}{2\tau^2} \sum_s \sum_{r \in \delta_s} (\gamma_s - \gamma_r)^2.$$

- Again yields a quadratic penalty

$$\text{pen}(\gamma|\tau^2) = \frac{1}{2\tau^2} \gamma' K \gamma.$$

- Kriging: Structured spatial effect.
- Assume a zero mean stationary Gaussian process for the spatial effect $\gamma_s = f_{spat}(s)$.
- Correlation of two sites is defined by an intrinsic correlation function.
- Can be interpreted as a basis function approach with radial basis functions.



- I.i.d. random effects: Unstructured spatial effect

$$\gamma_s \text{ i.i.d. } N(0, \tau^2).$$

- Also accounts for longitudinal structure of the data.
- Requires multiple measurements per observation plot.

Bayesian Inference

- All vectors of function evaluations f_j in the geoadditive predictor can be expressed as

$$f_j = Z_j \gamma_j$$

  with design matrix Z_j, constructed from the corresponding covariates, and regression coefficients γ_j.

- Each vector of regression coefficients follows a partially improper multivariate Gaussian prior:

$$p(\gamma_j|\tau_j^2) \propto \exp\left(-\frac{1}{2\tau_j^2}\gamma_j' K_j \gamma_j\right).$$

- The log-prior can be interpreted as a penalty term.

- The precision matrix K_j acts as a penalty matrix that ensures smoothness of the corresponding estimates.
- The variance τ_j^2 can be interpreted as a smoothing parameter and controls the trade-off between smoothness and fidelity to the data:
  - τ_j^2 small $\Rightarrow$ smooth estimates.
  - τ_j^2 large $\Rightarrow$ wiggly estimates.

- Fully Bayesian inference:
  - All parameters (including the variance parameters τ_j^2) are assigned suitable prior distributions.
  - Estimation is based on MCMC simulation techniques.
  - Usual estimates: Posterior expectation, posterior median (easily obtained from the samples).
- Empirical Bayes inference:
  - Differentiate between parameters of primary interest (regression coefficients) and hyperparameters (variances).
  - Assign priors only to the former.
  - Estimate the hyperparameters by maximising their marginal posterior.
  - Plugging these estimates into the joint posterior and maximising with respect to the parameters of primary interest yields posterior mode estimates.

Fully Bayesian inference based on MCMC

- Assign inverse gamma prior to τ_j^2:

$$p(\tau_j^2) \propto \frac{1}{(\tau_j^2)^{a_j+1}} \exp\left(-\frac{b_j}{\tau_j^2}\right).$$

Proper for	$a_j > 0,\ b_j > 0$	Common choice: $a_j = b_j = \varepsilon$ small.
Improper for	$b_j = 0,\ a_j = -1$	Flat prior for variance τ_j^2,
	$b_j = 0,\ a_j = -\frac{1}{2}$	Flat prior for standard deviation τ_j.

- Conditions for proper posteriors: Enough observations and either
  - proper priors for the variances or
  - $a_j < b_j = 0$ and rank deficiency in the prior for γ_j not too large.

- MCMC sampling scheme:
  - Metropolis-Hastings update for $\gamma_j|\cdot$:

    Propose new state from a multivariate Gaussian distribution with precision matrix and mean

    $$P_j = Z_j' W Z_j + \frac{1}{\tau_j^2} K_j \qquad \text{and} \qquad m_j = P_j^{-1} Z_j' W (\tilde{y} - \eta_{-j}).$$

    IWLS-Proposal with appropriately defined working weights W and working observations $\tilde{y}$.
  - Gibbs sampler for $\tau_j^2|\cdot$:

    Sample from an inverse Gamma distribution with parameters

    $$a_j' = a_j + \frac{1}{2}\text{rank}(K_j) \qquad \text{and} \qquad b_j' = b_j + \frac{1}{2}\gamma_j' K_j \gamma_j.$$

- Efficient algorithms make use of the sparse matrix structure of P_j and K_j.

Empirical Bayes inference based on mixed model methodology

- Consider the variances τ_j^2 as unknown constants to be estimated.
- Idea: Consider γ_j a correlated random effect with multivariate Gaussian distribution and use mixed model methodology.
- Problem: In most cases partially improper random effects distribution.
- Mixed model representation: Decompose

$$\gamma_j = X_j \beta_j + U_j b_j,$$

where

$$p(\beta_j) \propto const \qquad \text{and} \qquad b_j \sim N(0, \tau_j^2 I_{k_j}).$$

$\Rightarrow$ β_j is a fixed effect and b_j is an i.i.d. random effect.

- This yields the variance components model

$$\eta = x'\beta + u'b,$$

where in turn

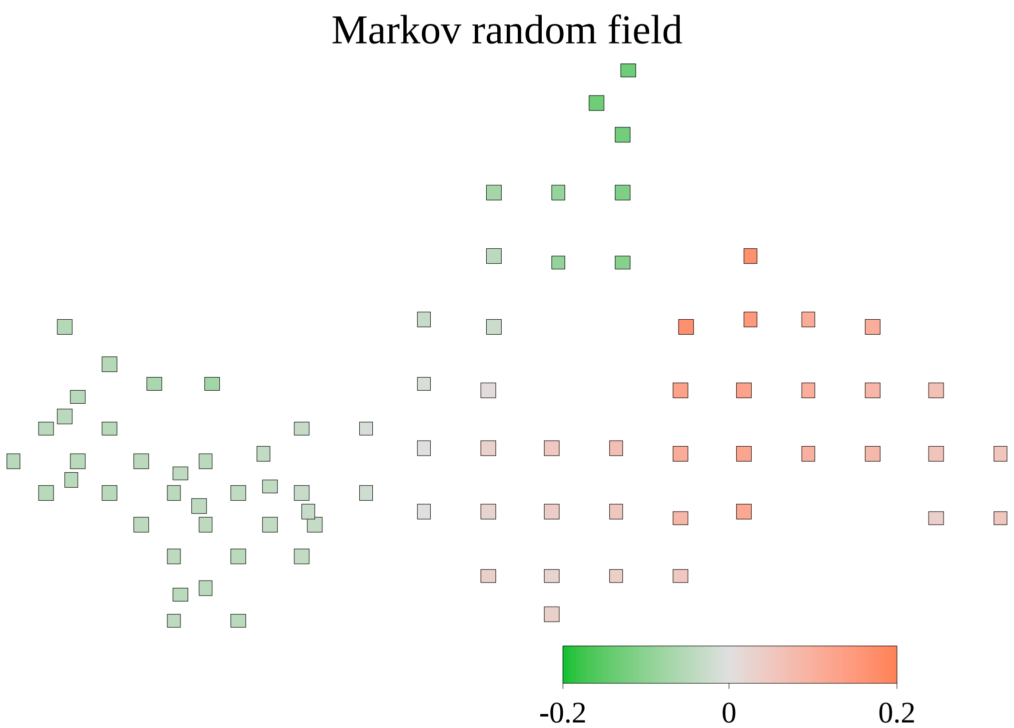
$$p(\beta) \propto const \qquad \text{and} \qquad b \sim N(0, Q).$$

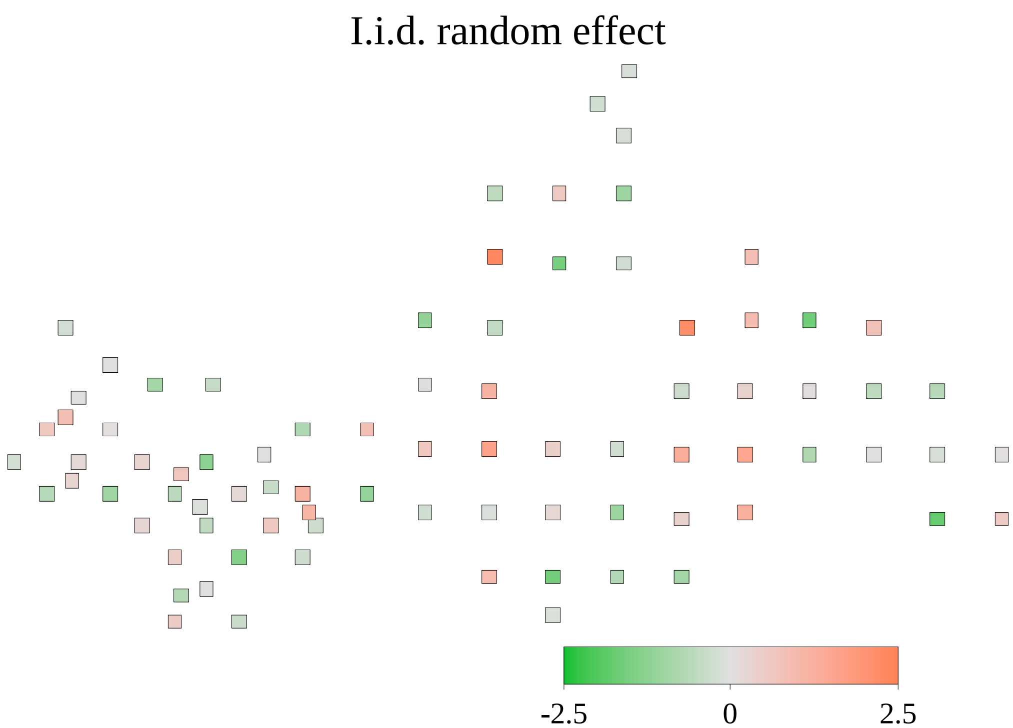
- Obtain empirical Bayes estimates / penalized likelihood estimates via iterating
  - Penalized maximum likelihood for the regression coefficients β and b.
  - Restricted maximum / marginal likelihood for the variance parameters in Q:

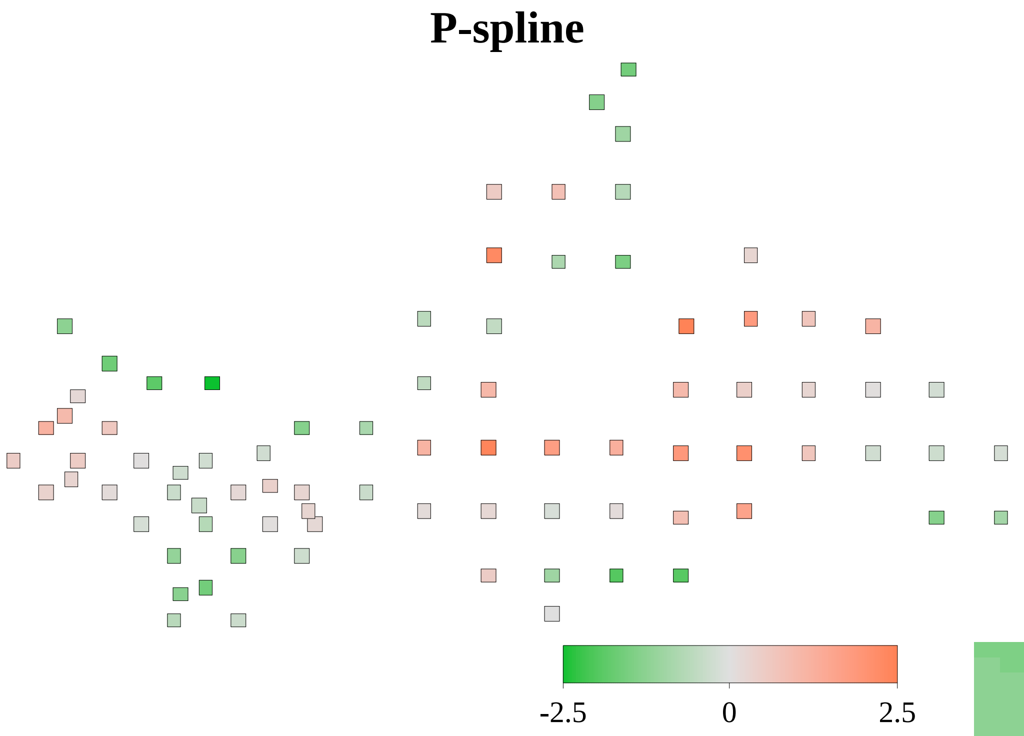
$$L(Q) = \int L(\beta, b, Q) p(b) d\beta db \to \max_Q .$$

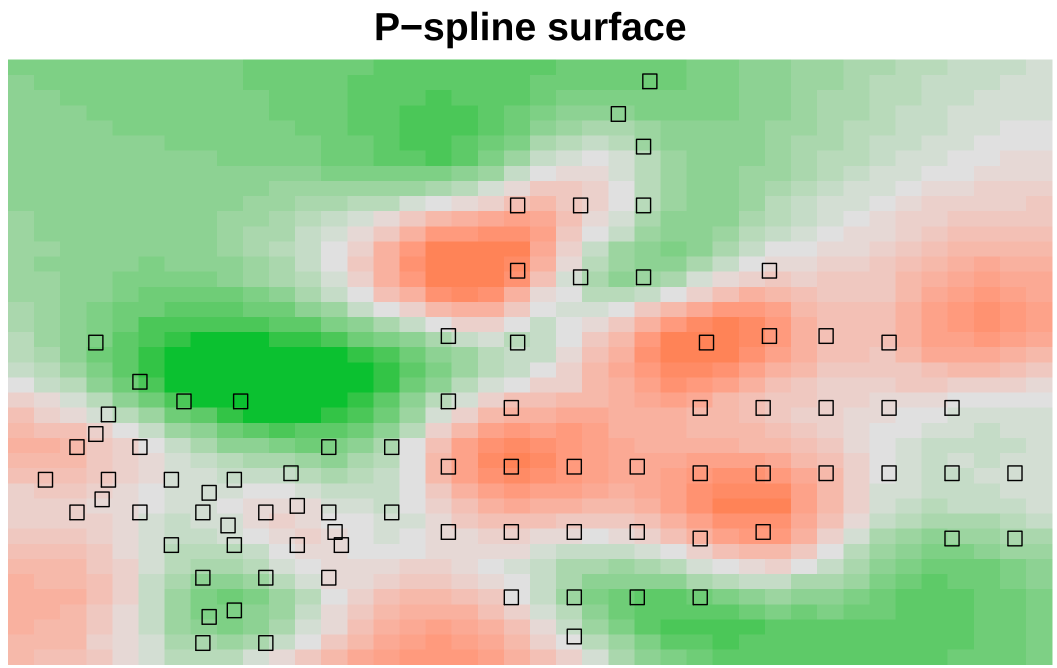
- Involves Laplace approximation to the marginal likelihood.
- Corresponds to REML estimation of variances in Gaussian mixed models.

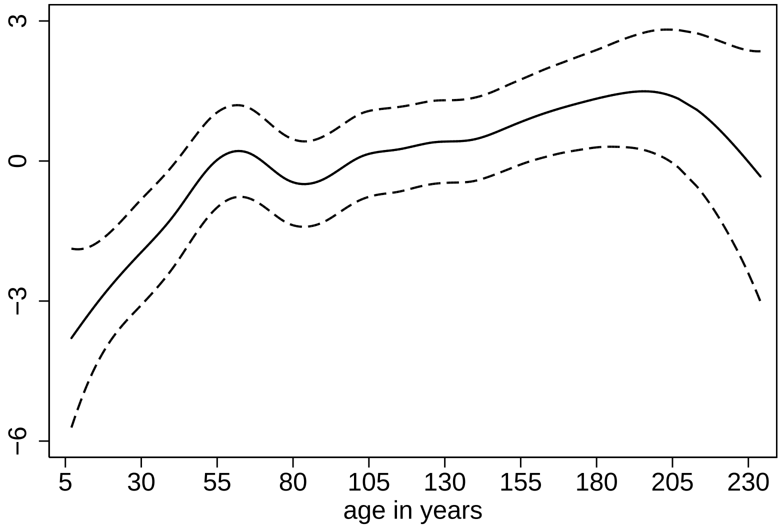
Results

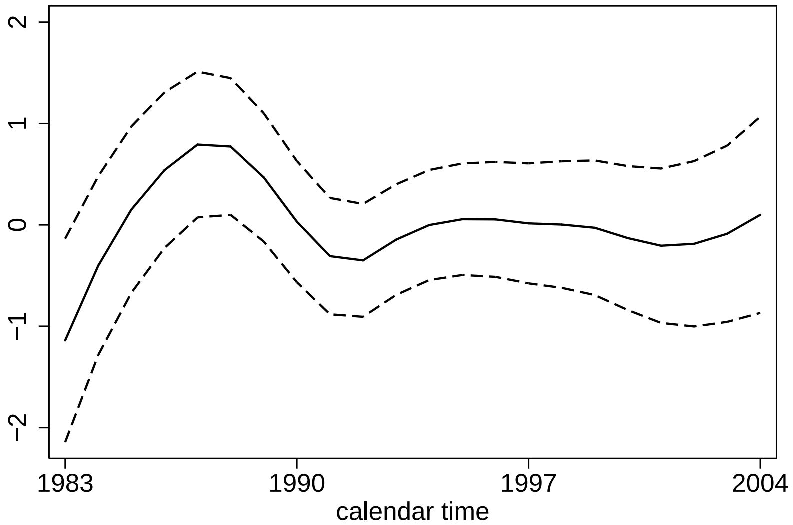


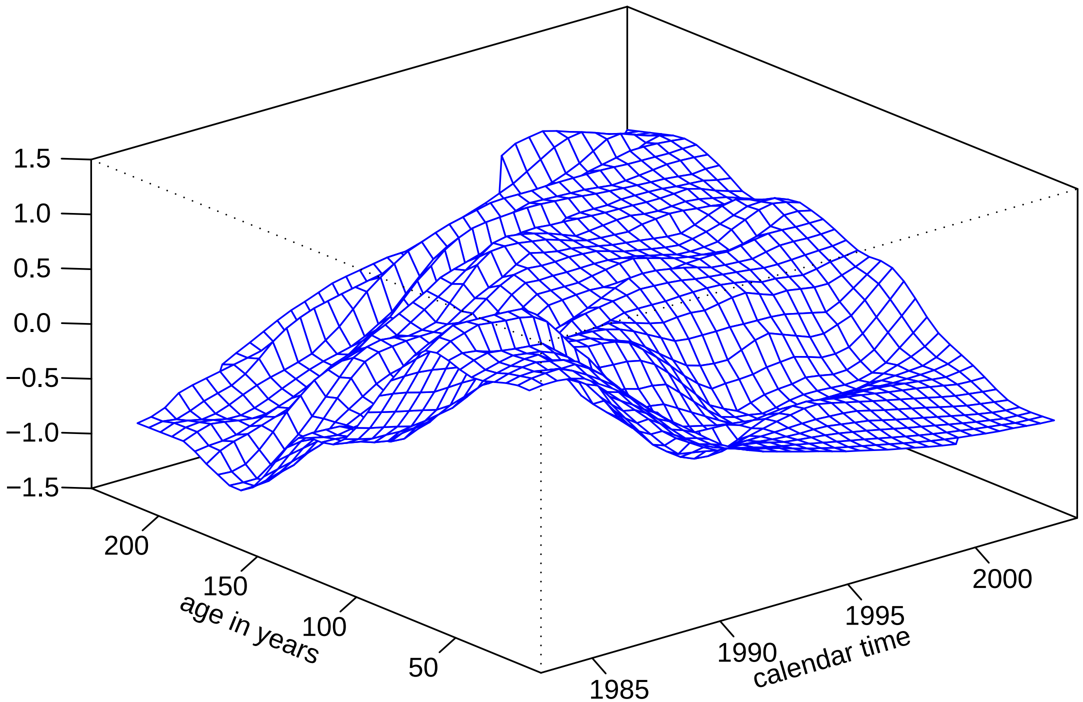


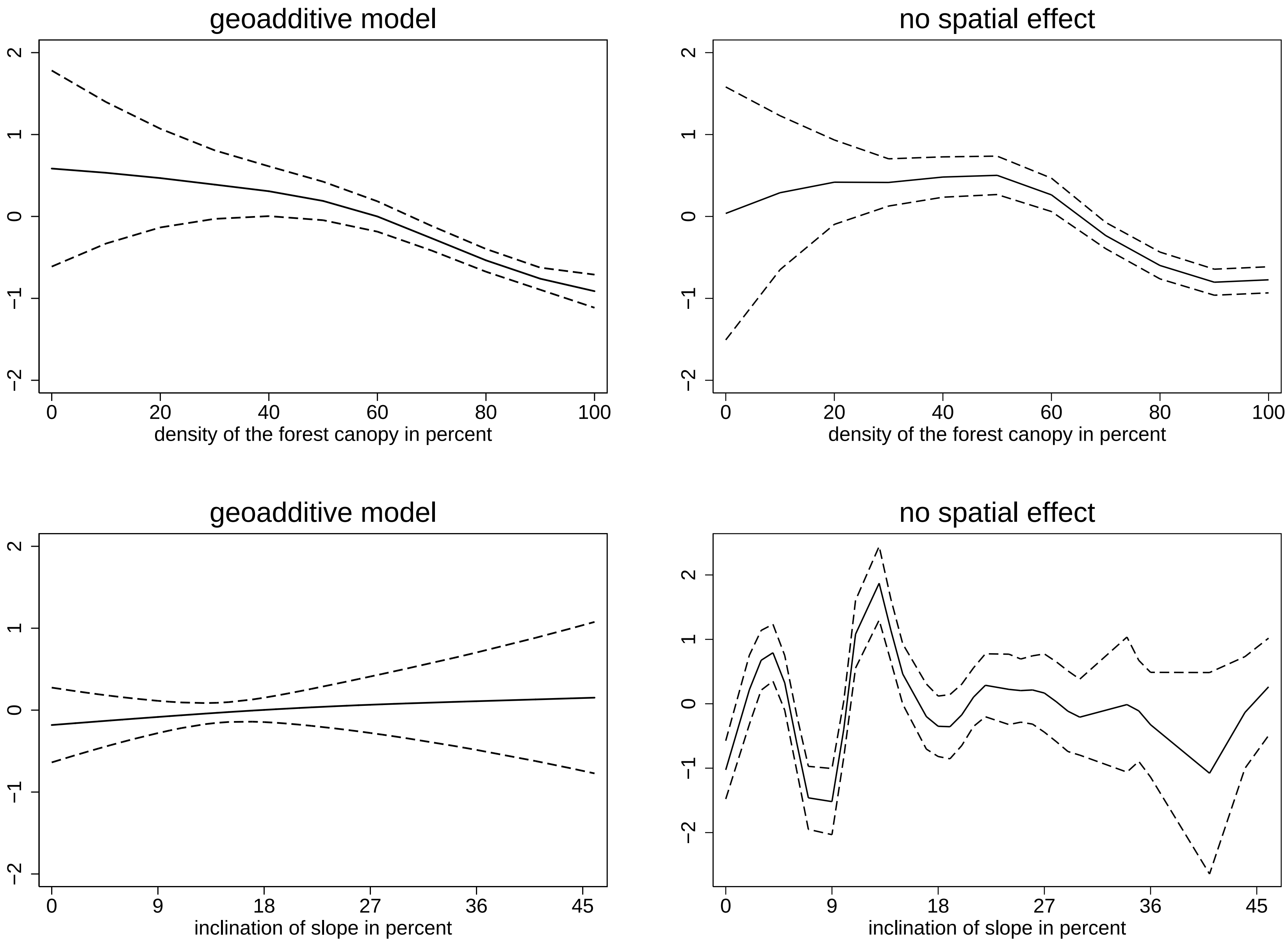

P-spline
-2.5
0
2.5


P−spline surface


3
0
−3
−6
5
30
55
80
105
130
155
180
205
230
age in years


2
1
0
−1
−2
1983
1990
1997
2004
calendar time

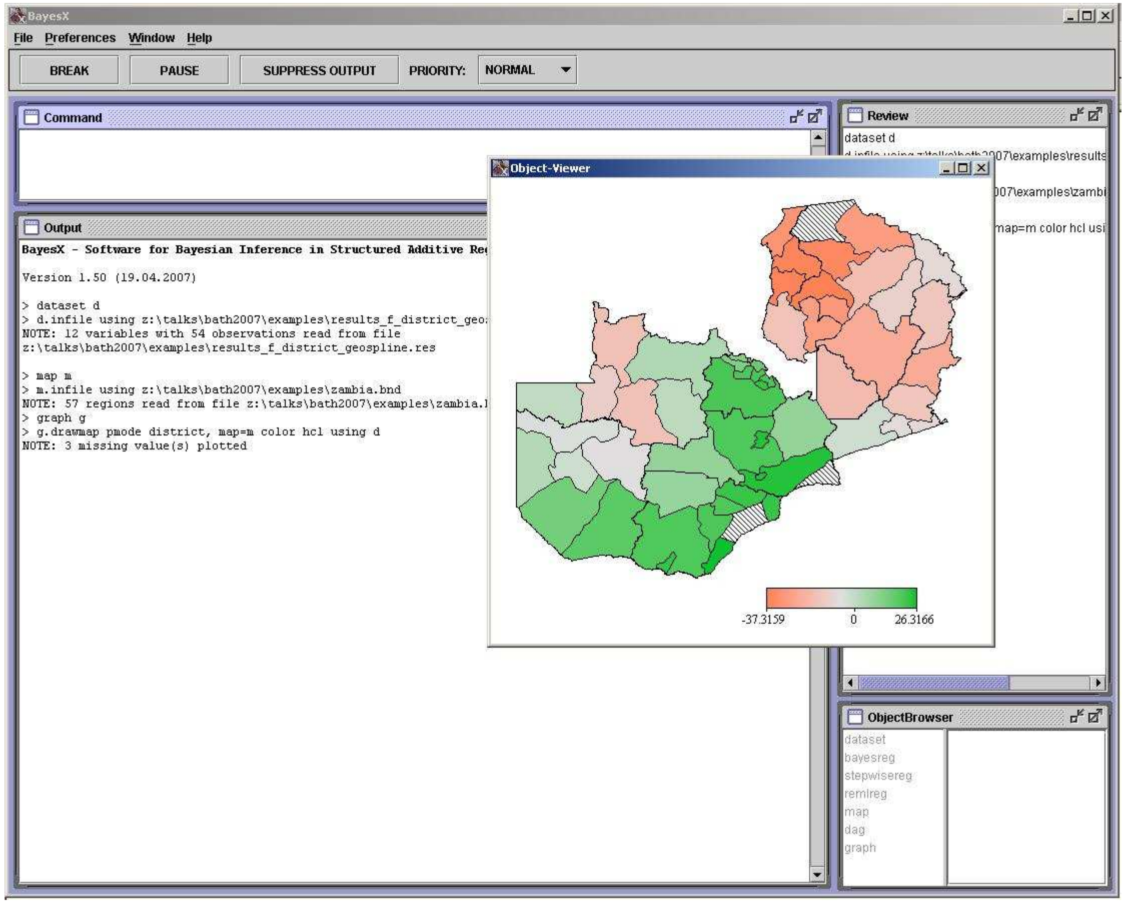

1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
200
150
100
50
age in years
1985
1990
1995
2000
calendar time


geoadditive model
no spatial effect
density of the forest canopy in percent
density of the forest canopy in percent
geoadditive model
no spatial effect
inclination of slope in percent
inclination of slope in percent
0
20
40
60
80
100
0
9
18
27
36
45
−2
−1
0
1
2

- Summary:
  - Inclusion of any kind of spatial effect leads to a dramatically improved model fit.
  - The unstructured part dominates the structured spatial effect.
  - Temporal effects are present in the data.
  - Nonparametric effects allow for more realistic models and additional insight.
  - Inclusion of the spatial effect also improved interpretability of other effects.

BayesX

- BayesX is a software tool for estimating geoadditive regression models.



- Stand-alone software with Stata-like syntax.
- Developed by Christiane Belitz, Andreas Brezger, Thomas Kneib and Stefan Lang with contributions of seven colleagues.
- Computationally demanding parts are implemented in C++.
- For Windows, a graphical user interface has been implemented in Java.
- The command line version of BayesX is platform independent.
- There is a supplementary R-package for easy visualisation of estimation results and for manipulating geographical information.
- More information:

`http://www.stat.uni-muenchen.de/~bayesx`

- Inferential procedures:
  - Fully Bayesian inference based on MCMC.
  - Empirical Bayes inference based on mixed model methodology.
  - Stepwise model selection procedures.
- Univariate response types:
  - Gaussian,
  - Bernoulli and Binomial,
  - Poisson and zero-inflated Poisson,
  - Gamma,
  - Negative Binomial.

- Categorical responses with ordered categories:
  - Ordinal as well as sequential models,
  - Logit and probit models,
  - Effects can be category-specific or constant over the categories.
- Categorical responses with unordered categories:
  - Multinomial logit and multinomial probit models,
  - Category-specific and globally-defined covariates,
  - Non-availability indicators can be defined to account for varying choice sets.

- Continuous survival times:
  - Cox-type hazard regression models,
  - Joint estimation of baseline hazard rate and covariate effects,
  - Time-varying effects and time-varying covariates,
  - Arbitrary combinations of right, left and interval censoring as well as left truncation.
- Multi-state models:
  - Describe the evolution of discrete phenomena in continuous time,
  - Model in terms of transition intensities, similar as in the Cox model.

Conclusions

- Take home messages: Spatio-temporal models
  - allow for sufficient flexibility in complex applications.
  - can be estimated for various types of responses.
  - can be estimated with automatic determination of smoothing parameters without the need for subjective judgements.
- Not in this talk: Model choice and variable selection in spatio-temporal regression models can be accomplished with boosting techniques.

- More on the application:

  Kneib, T. & Fahrmeir, L. (2010): A Space-Time Study on Forest Health. In: Chandler, R. E. & Scott, M. (eds.): Statistical Methods for Trend Detection and Analysis in the Environmental Sciences, Wiley.

- A place called home:

  `http://www.staff.uni-oldenburg.de/thomas.kneib`