

# Penalized structured additive regression for multicategorical space-time data

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joint work with Ludwig Fahrmeir and Stefan Lang

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## Forest health data

- Data collected in yearly forest health inventories carried out in a forest in northern Bavaria from 1983 to 2001.
- 83 observation points with beeches in an area extending 15 km from east to west and 10 km from north to south.
- $y_{it}$ , the defoliation degree of beech  $i$  in year  $t$ , is measured in three **ordered categories** (multicategorical response):
  - $y_{it} = 1$  no defoliation,
  - $y_{it} = 2$  defoliation 25% or less,
  - $y_{it} = 3$  defoliation above 25%.
- Covariates:
  - $t$  calendar time,
  - $s_i$  site of the beech,
  - $a_{it}$  age of the tree in years,
  - $u_{it}$  further (mostly categorical) covariates.

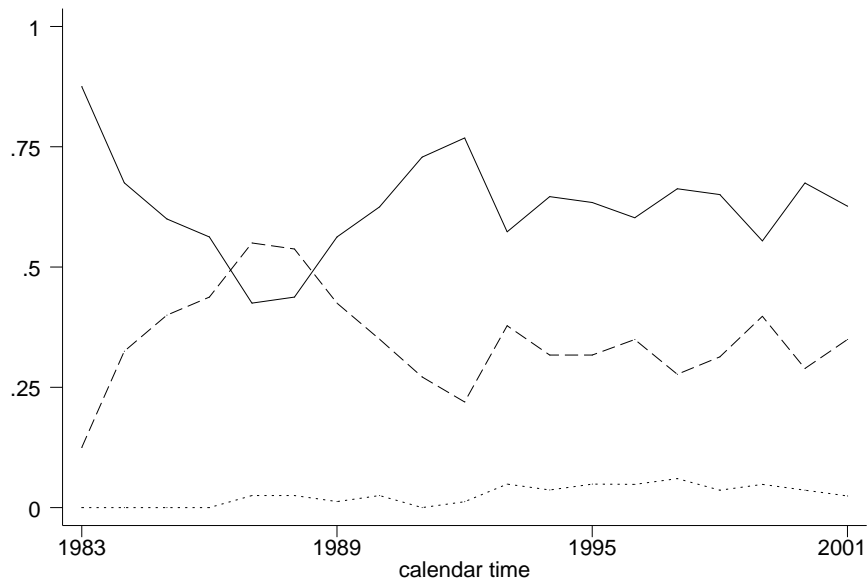
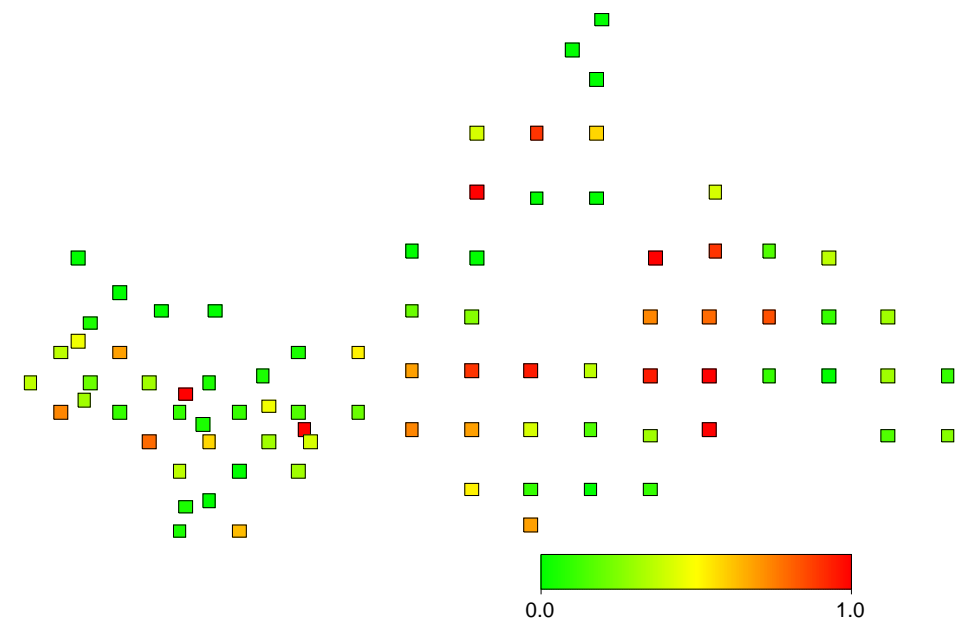


Figure 1: Temporal development of the frequency of the damage states:

- no damage,
- - - medium damage,
- ... severe damage.

Figure 2: Spatial distribution of the beeches and percentage of time points for which a beech was classified to be damaged (damage state 2 or 3).



## Multicategorical models for ordinal response

- Response  $y_{it}$  follows multinomial distribution with three ordered categories  $r = 1, 2, 3$ .
- Model the **cumulative probabilities**

$$P(y_{it} \leq r) = F(\theta_r - \eta_{it})$$

with thresholds  $-\infty = \theta_0 < \theta_1 < \theta_2 < \theta_3 = \infty$  and linear predictor  $\eta_{it}$ .

- $F(\cdot)$  can be any cumulative distribution function:
  - standard normal  $\implies$  cumulative **probit** model,
  - logistic  $\implies$  cumulative **logit** model.

- Consider a random variable with density  $f = F'$  and expectation  $\eta_{it}$ .

⇒ Linear predictor determines shift on latent scale.

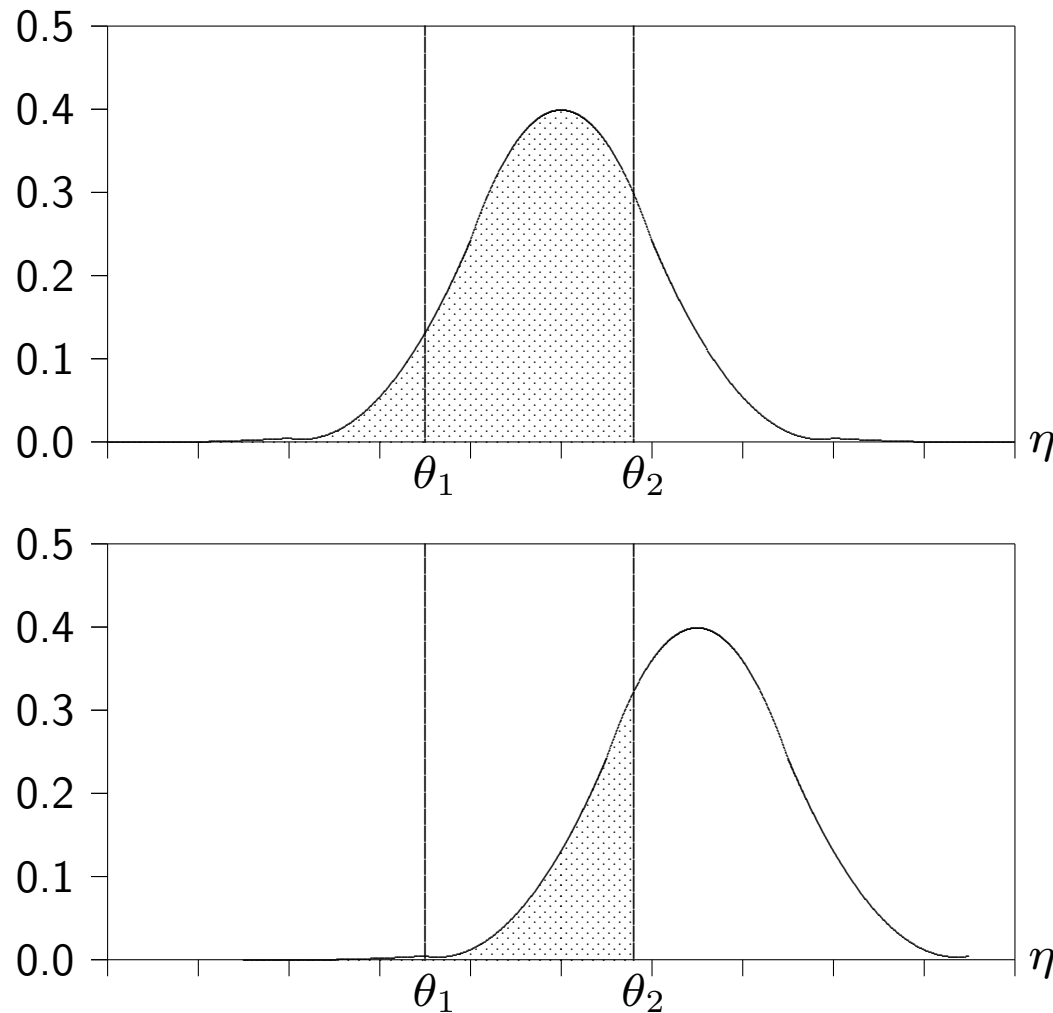


Figure 3: The shaded areas represent  $P(y_{it} \leq 2)$  for different values of  $\eta_{it}$ .

- Limitations of a purely parametric approach:
    - Spatio-temporal structure of the data implies **spatial** and **temporal correlations**.
    - **Nonlinear effects** of continuous covariates?
    - **Complex interactions** between covariates?
- ⇒ Structured additive regression models.

## Penalized structured additive regression

- Replace usual **parametric** predictor with a **flexible semiparametric** predictor

$$\eta_{it} = f_1(t) + f_2(a_{it}) + f_3(t, a_{it}) + f_{spat}(s_i) + u'_{it}\gamma,$$

where

- $f_1$  and  $f_2$  are **nonparametric** functions of calendar time and age,
  - $f_3$  is an **interaction surface** between calendar time and age,
  - $f_{spat}$  is a **spatial** function, and
  - $u$  is a vector of further covariates with parametric effects.
- Structured additive regression extends (and combines) generalized additive mixed models, geospatial models and varying coefficient models.
  - Allows **unified treatment** of all effects within a **Bayesian framework**.

- $f_1(t), f_2(a_{it})$ : **P-splines**
  - Approximate  $f_j$  by a B-spline of a certain degree (basis function approach).
  - Penalize differences between adjacent parameters of basis functions to ensure smoothness.
  - Alternatives: Random walks, autoregressive priors.
- $f_3(t, a_{it})$ : **Two-dimensional extensions of P-splines**
  - Define two-dimensional basis functions based on tensor products of one-dimensional B-splines.
  - Use priors from spatial statistics for penalization.
  - Alternative: Varying coefficient models, if one of the interacting variables is categorical.



- $f_{spat}(s_i)$ : **Markov random fields**
  - Consider two trees as neighbors if their distance is less than (e.g.) 1.2 km.
  - Assume that the expected value of  $f_{spat}(s)$  is the average of the function evaluations of adjacent sites.
- $f_{spat}(s_i)$ : **Stationary Gaussian random fields** (kriging)
  - Spatial effect follows a zero mean stationary Gaussian stochastic process.
  - Correlation of two arbitrary sites is defined by an intrinsic correlation function.
- Split up spatial effect into **structured** and **unstructured** part. The unstructured effect can be modelled by i.i.d. random effects, the structured effect by a MRF or a GRF.

## Mixed model representation

- All nonparametric effects can be expressed as the product of a **design matrix**  $Z$  and a vector of **regression coefficients**  $\beta$ .
- Rewrite the structured additive predictor in matrix notation as

$$\eta = Z_1\beta_1 + Z_2\beta_2 + Z_3\beta_3 + Z_{spat}\beta_{spat} + U\gamma.$$

- Bayesian approach: Assign an appropriate **prior** to  $\beta_j$ .
- All priors can be cast into the **general form**

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

where  $K_j$  is a **penalty matrix** and  $\tau_j^2$  is a **smoothing parameter**.

- Type of the covariate and prior beliefs about the smoothness of  $f_j$  determine special  $Z_j$  and  $K_j$ .

- Accuracy of the estimation relies heavily on the choice of the smoothing parameters.
- Idea: Reexpress the structured additive regression model as a **multicategorical mixed model** and use **mixed model methodology**.
- Each parameter vector  $\beta_j$  can be partitioned into an **unpenalized part** (with flat prior) and a **penalized part** (with i.i.d. Gaussian prior) yielding a **variance components model**

$$\eta = X^{unp} \beta^{unp} + X^{pen} \beta^{pen}$$

with

$$p(\beta^{unp}) \propto \text{const} \quad \beta^{pen} \sim N(0, \Lambda)$$

and

$$\Lambda = \text{blockdiag}(\tau_1^2 I, \dots, \tau_4^2 I).$$

- Regression coefficients are estimated via **modified Fisher scoring**.
- The mixed model representation allows for **restricted maximum likelihood / marginal likelihood** estimation of the variance components:

$$L(\Lambda) = \int L(\beta^{unp}, \beta^{pen}, \Lambda) p(\beta^{pen}) d\beta^{pen} d\beta^{unp} \rightarrow \max_{\Lambda}.$$

- From a Bayesian perspective, we get **empirical Bayes / posterior mode** estimates.
- Closely related to penalized likelihood.
- Fahrmeir, Kneib and Lang (2004) derive numerically efficient formulae that allow the computation even for fairly large data sets.

# Results

Figure 4: Time trend.

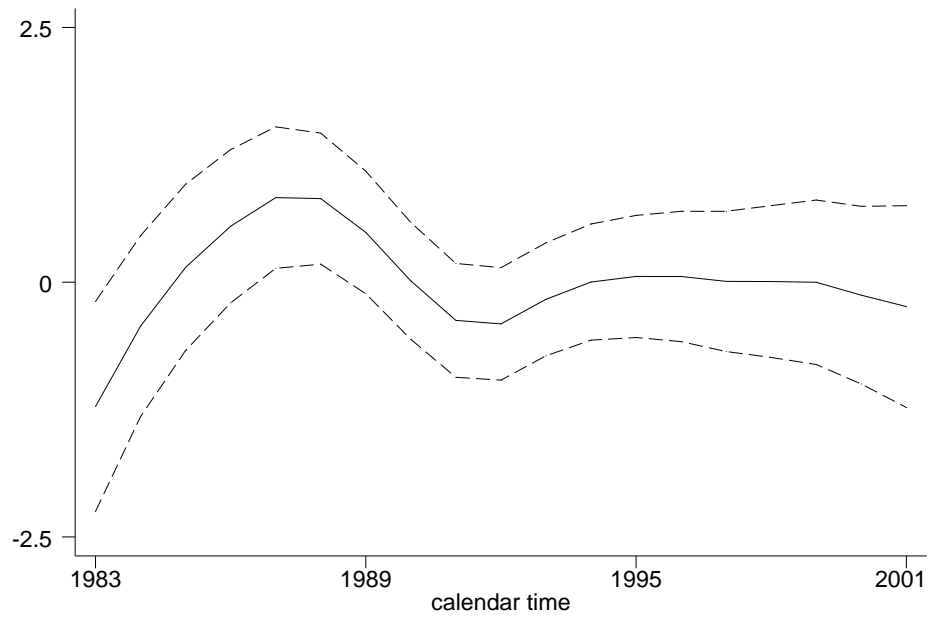
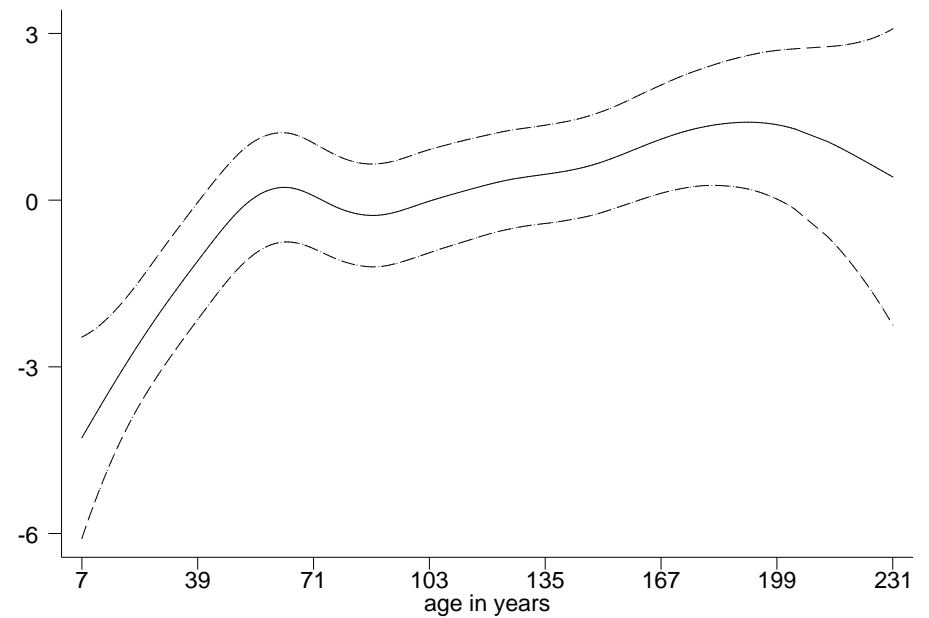


Figure 5: Age effect.



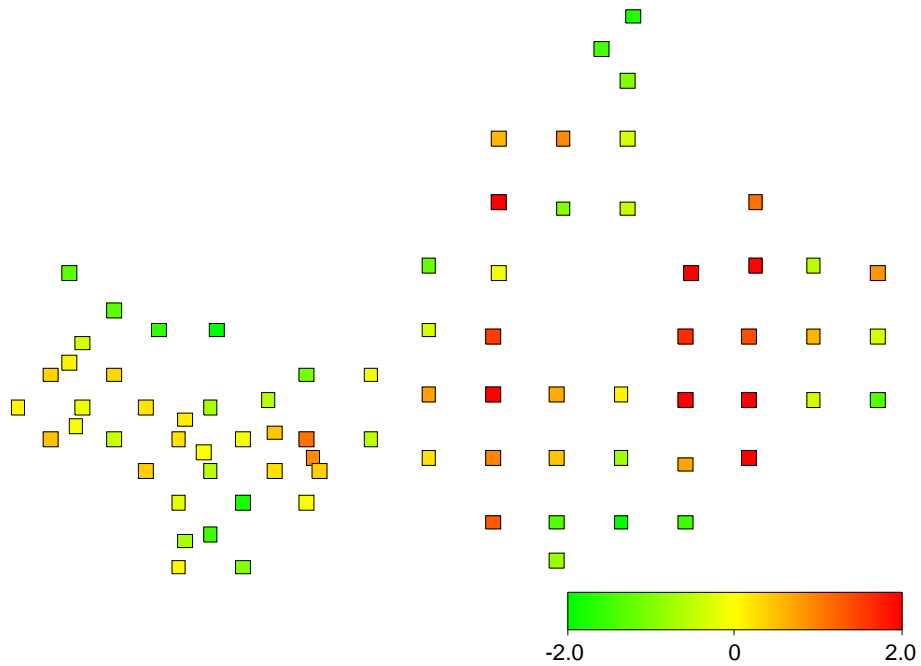


Figure 6: Structured spatial effect.

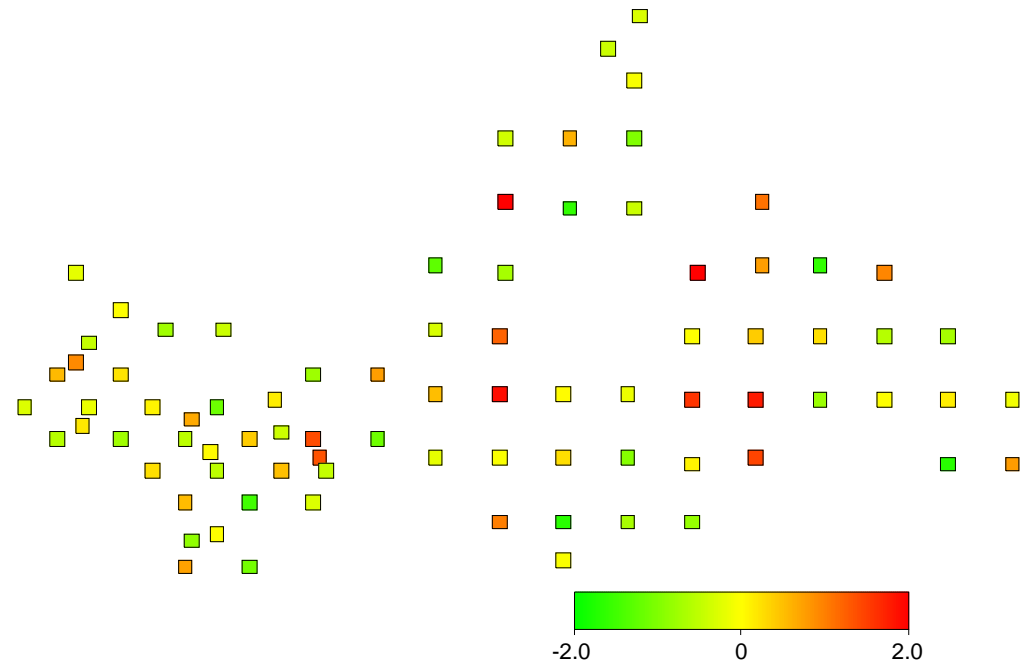


Figure 7: Unstructured spatial effect.

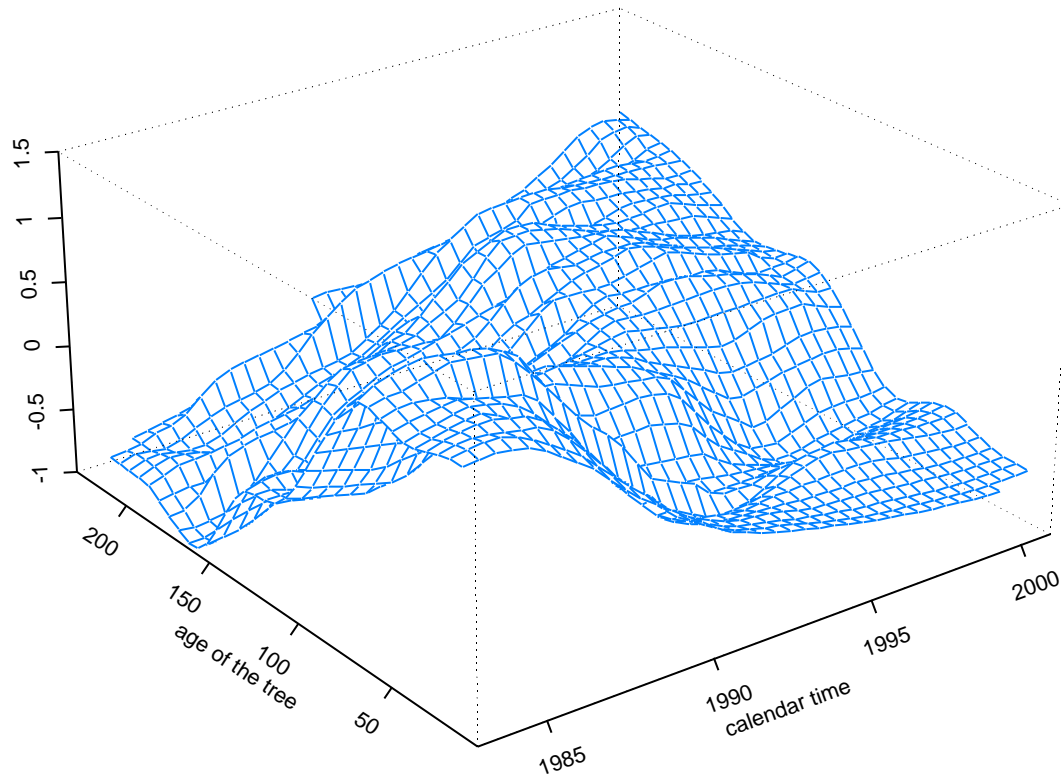


Figure 8: Interaction effect.

Table 1: Classifications with and without spatial effect.

$y$	$\hat{y}$		
	1	2	3
1	904	64	0
2	108	426	5
3	0	16	24

12.5%

$y$	$\hat{y}$		
	1	2	3
1	850	118	0
2	150	386	3
3	0	34	6

19.7%

## Software

- Estimation was carried out using BayesX, a public domain software package for Bayesian inference.



- Available from

<http://www.stat.uni-muenchen.de/~lang/bayesx>



- Features (within a mixed model setting):
  - Responses: Gaussian, Gamma, Poisson, Binomial, ordered and unordered multinomial.
  - Continuous covariates and time scales: Random Walks, P-splines, autoregressive priors for seasonal components.
  - Spatial Covariates: Markov random fields, stationary Gaussian random fields, two-dimensional P-Splines.
  - Interactions: two-dimensional P-splines, varying coefficient models with continuous and spatial effect modifiers.
  - Random intercepts and random slopes.

## References

- Fahrmeir, L., Kneib, T. and Lang, S. (2004): Penalized structured additive regression for space-time data: A Bayesian perspective. Under revision for *Statistica Sinica*.
- Kneib, T. and Fahrmeir, L. (2004): Structured additive regression for multicategorical space-time data: A mixed model approach. SFB 386 Discussion Paper 377, University of Munich.
- Both available from

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