

Structured Additive Regression Models: An R Interface to BayesX

Nikolaus Umlauf Thomas Kneib Stefan Lang Achim Zeileis
Universität Innsbruck Universität Oldenburg Universität Innsbruck Universität Innsbruck

Abstract

Structured additive regression (STAR) models provide a flexible framework for modeling possible nonlinear effects of covariates: They contain the well established frameworks of generalized linear models (GLM) and generalized additive models (GAM) as special cases but also allow a wider class of effects, e.g. for geographical or spatio-temporal data. This allows to specify complex and realistic models that can be estimated using Bayesian inference based on modern Markov chain Monte Carlo (MCMC) simulation techniques, based on a mixed model representation of STAR models, or with stepwise regression techniques combining penalized least squares estimation with model selection. Software for fitting STAR models is provided in the standalone software package **BayesX**: a comprehensive open-source regression toolbox written in C++ code. **BayesX** not only covers models for responses from univariate exponential families, but also models from less-standard regression situations such as models for multi-categorical responses with either ordered or unordered categories, continuous time survival data, or continuous time multi-state models. This paper presents the full interactive R interface **R2BayesX** to **BayesX**. With the new package, STAR models can be conveniently specified using R's formula language (with some extended terms), fitted using the **BayesX** binary, represented in R with objects of suitable classes, and finally printed/summarized/plotted. As a result of the superior graphics capabilities of R package **R2BayesX** greatly enhances the usability of **BayesX**. On the other hand some of the more complex models from the STAR class, especially models for multivariate responses, extend the already impressive capabilities for semiparametric regression in R. Moreover, **R2BayesX** is the most comprehensive package for simulation based Bayesian semiparametric regression in R.

Keywords: STAR models, MCMC, REML, stepwise, R.

1. Introduction

The free software **BayesX** (Brezger, Kneib, and Lang 2005) is a standalone program comprising powerful tools for Bayesian and mixed model based inference in complex semiparametric regression models with structured additive predictor (STAR, see Section 3). To gain improved computational performance, the algorithms implemented utilize numerically efficient (sparse) matrix architectures and are written in a C++ environment. Besides exponential family regression, **BayesX** also supports models for multi-categorical responses, hazard regression for continuous survival times, and continuous time multi-state models.

In this article, we describe the full interactive R (R Development Core Team 2011) interface to the command-line binary version of BayesX, which is an extension of package **BayesX**

(Kneib, Heinzl, Brezger, and Sabanes Bove 2011), that mainly provides functionality for exploring estimation results. The R package is called **R2BayesX** and has recently been added to the Comprehensive R Archive Network (CRAN, <http://CRAN.R-project.org/package=R2BayesX>). Within the new package, users are now provided with a typical R front end that may

- specify and estimate STAR models with **BayesX** directly from the console (function `bayesx()`, Section 5.3),
- apply a set of extractor functions and methods on **BayesX** fitted model objects, e.g. producing high level graphics of estimated effects, model diagnostic plots, summary statistics and more (Table 3),

In addition, users can

- run already existing **BayesX** input program files from R (function `run.bayesx()`, Section 5.5),
- automatically import **BayesX** output files into R (function `read.bayesx.output()`, Section 5.5).

Furthermore, the models supported by **BayesX** are conveniently specified using R's formula language definition, wherefore several special model term constructor functions, such as the main **R2BayesX** constructor functions `sx()` and `r()` for smooth and random effects, respectively, as well as the functions `s()` and `te()` from the **mgcv** package (Wood 2011b, 2006), facilitate a consistent way to translate R syntax into **BayesX** interpretable commands (see Section 5.4).

The reminder of this paper is as follows. The next section gives a first example of a common R session applying **R2BayesX** on a dataset on childhood malnutrition in Zambia. Section 3 briefly discusses the methodological background of regression models with a structured additive predictor, before a description on implementation details and the user interface is given in Section 4 and 5 respectively. In Section 6, the interface usability is further illustrated with the childhood malnutrition data and a dataset on forest health.

2. Motivating example

To give an introductory example of the various features of the interface, we estimate a Bayesian geoadditive regression model for the childhood malnutrition dataset in Zambia (see Section 6.1, Kandala, Lang, Klasen, and Fahrmeir 2001) using Markov chain Monte Carlo (MCMC) simulation.

The data consists of 4847 observations including 8 variables, both continuous and categorical. In this analysis, the main interest is on modeling the dependence of stunting (`stunting`), represented by anthropometric indicators of newborn children, on covariates including the age of the child (`age`), the body mass index of the mother (`mbmi`) and the district the child lives in (`district`). The model is given by

$$\text{stunting}_i = \gamma_0 + f_1(\text{agechild}_i) + f_2(\text{mbmi}_i) + f_{\text{spat}}(\text{district}_i) + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2),$$

where the functions f_1 and f_2 of continuous covariates `agechild` and `mbmi` have possible nonlinear effects on `stunting` and are modeled nonparametrically using P(enalized)-splines. Here, the spatially correlated effect f_{spat} of locational covariate `district` is modeled using Kriging based on centroid coordinates (geokriging) of the districts in Zambia. To estimate the model with **BayesX** from R, the data together with a boundary map file of the districts in Zambia is loaded with

```
R> data("ZambiaNutrition", "ZambiaBnd", package = "R2BayesX")
```

Boundary files are basically shapefiles (see also package **shapefiles**, [Stabler 2006](#)) that only include information on the polygons that form the map and may be constructed using function `shp2bnd()` or imported with `read.bnd()`. The model formula is specified by

```
R> f <- stunting ~ sx(agechild) + sx(mbmi) +
+   sx(district, bs = "gk", map = ZambiaBnd, full = TRUE)
```

Finally, the model is fitted with the main model-fitting function `bayesx()`

```
R> b <- bayesx(f, family = "gaussian", method = "MCMC",
+   data = ZambiaNutrition)
```

Thereafter, a model summary is displayed by calling

```
R> summary(b)
```

Call:

```
bayesx(formula = f, data = ZambiaNutrition, family = "gaussian",
  method = "MCMC")
```

Fixed effects estimation results:

Parametric Coefficients:

	Mean	Sd	2.5%	50%	97.5%
(Intercept)	0.0252	0.0403	-0.0560	0.0273	0.1032

Smooth terms variances:

	Mean	Sd	2.5%	50%	97.5%	Min	Max
sx(agechild)	0.0064	0.0067	0.0012	0.0043	0.0246	0.0007	0.0688
sx(district)	0.0449	0.0178	0.0206	0.0410	0.0905	0.0111	0.1256
sx(mbmi)	0.0021	0.0035	0.0003	0.0012	0.0094	0.0002	0.0501

Scale estimate:

	Mean	Sd	2.5%	50%	97.5%
Sigma2	0.8172	0.0161	0.7872	0.8171	0.8499

```
N = 4847 burnin = 2000 DIC = 4888.096 pd = 37.91711
method = MCMC family = gaussian iterations = 12000 step = 10
```

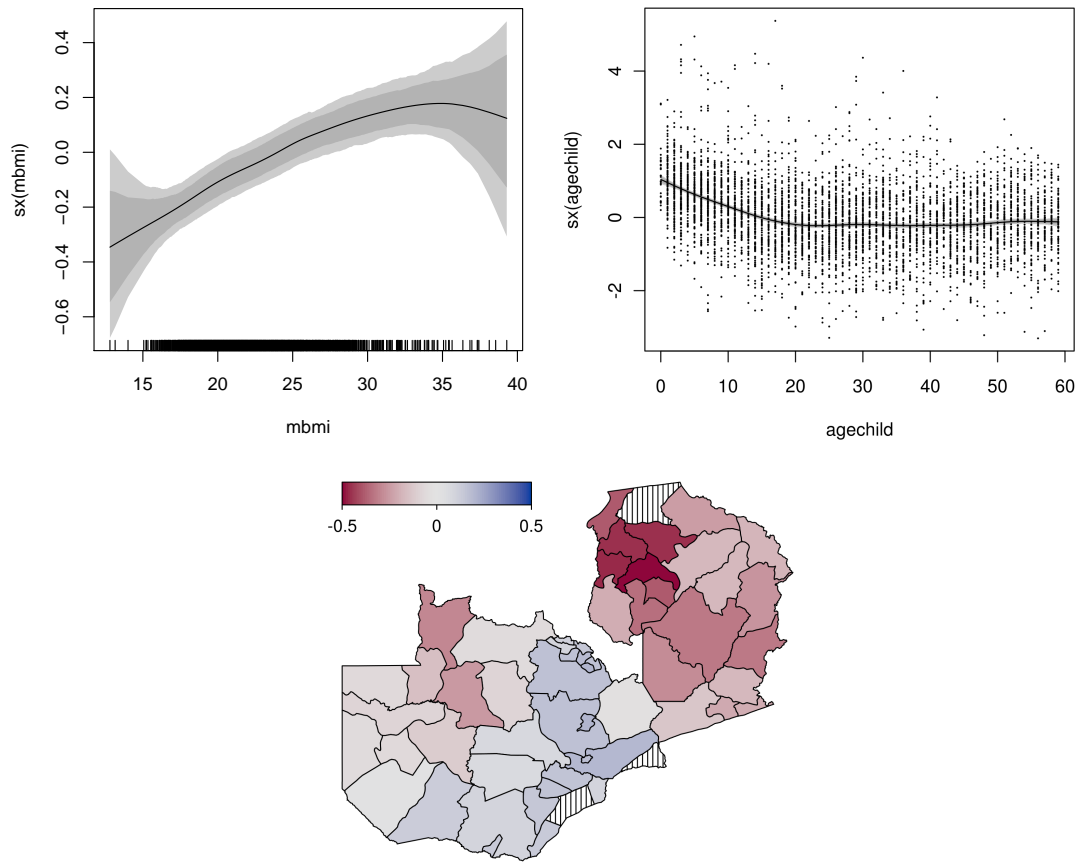


Figure 1: Visualization examples: Estimated effect for covariate **mbmi** (black line) together with 95% and 80% credible intervals (upper left panel). The upper right panel shows the estimated effect of **agechild** including partial residuals. The lower panel illustrates visualization of the estimated spatial effect for covariate **district** using a map effect plot.

A plot of the estimated effect for covariate **mbmi** may then be produced by typing

```
R> plot(b, term = "sx(mbmi)")
```

and for covariate **agechild** including partial residuals by

```
R> plot(b, term = "sx(agechild)", residuals = TRUE)
```

The estimated effect of the correlated spatial effect of the districts in Zambia may e.g. be visualized using a map effect plot generated by

```
R> plot(b, term = "sx(district)", map = ZambiaBnd)
```

The plots are shown in Figure 1.

3. STAR models

The STAR model class supported by **R2BayesX** is based on the framework of Bayesian generalized linear models (GLM) (e.g. see [Fahrmeir, Kneib, and Lang 2009](#) and [Fahrmeir and Tutz 2001](#)). GLMs assume that, given covariates \mathbf{x} and unknown parameters $\boldsymbol{\gamma}$, the distribution of the response variable y belongs to an exponential family with mean $\mu = E(y|\mathbf{x}, \boldsymbol{\gamma})$ linked to a linear predictor η by

$$\mu = h^{-1}(\eta), \quad \eta = \mathbf{x}'\boldsymbol{\gamma},$$

where h is a known link function and $\boldsymbol{\gamma}$ are unknown regression coefficients. In STAR models ([Fahrmeir, Kneib, and Lang 2004](#); [Brezger and Lang 2006](#)), the linear predictor is replaced by a more general and flexible, structured additive predictor

$$\eta = f_1(\mathbf{z}) + \dots + f_p(\mathbf{z}) + \mathbf{x}'\boldsymbol{\gamma}, \quad (1)$$

with $\mu = E(y|\mathbf{x}, \mathbf{z}, \boldsymbol{\gamma}, \boldsymbol{\theta})$ and \mathbf{z} represents a generic vector of all nonlinear modeled covariates. The vector $\boldsymbol{\theta}$ comprises all parameters of the functions f_1, \dots, f_p . The functions f_j are possibly smooth functions comprising effects as e.g. given by

- nonlinear effects of continuous covariates: $f_j(\mathbf{z}) = f(z_1)$,
- two-dimensional surfaces: $f_j(\mathbf{z}) = f(z_1, z_2)$,
- spatially correlated effects: $f_j(\mathbf{z}) = f_{spat}(z_s)$,
- varying coefficients: $f_j(\mathbf{z}) = z_1 f(z_2)$,
- spatially varying effects: $f_j(\mathbf{z}) = z_1 f_{spat}(z_s)$ or $f_j(\mathbf{z}) = z_1 f(z_2, z_3)$,
- random intercepts with cluster index c : $f_j(\mathbf{z}) = \beta_c$,
- random slopes with cluster index c : $f_j(\mathbf{z}) = z_1 \beta_c$.

STAR models cover a number of well known model classes as special cases, including generalized additive models (GAM, [Hastie and Tibshirani 1990](#)), generalized additive mixed models (GAMM, [Lin and Zhang 1999](#)), geoadditive models ([Kamman and Wand 2003](#)), varying coefficient models ([Hastie and Tibshirani 1993](#)), and geographically weighted regression ([Fotheringham, Brunsdon, and Charlton 2002](#)).

The unified representation of a STAR predictor arises from the fact that all functions f_j in (1) may be specified by a basis function approach, where the vector of function evaluations $\mathbf{f}_j = (f_j(\mathbf{z}_1), \dots, f_j(\mathbf{z}_n))$ of the $i = 1, \dots, n$ observations can be written in matrix notation

$$\mathbf{f}_j = \mathbf{Z}_j \boldsymbol{\beta}_j,$$

where the design matrix \mathbf{Z}_j depends on the specific term structure chosen for f_j and $\boldsymbol{\beta}_j$ are unknown regression coefficients to be estimated. Hence, the predictor (1) may be rewritten as

$$\boldsymbol{\eta} = \mathbf{Z}_1 \boldsymbol{\beta}_1 + \dots + \mathbf{Z}_p \boldsymbol{\beta}_p + \mathbf{X} \boldsymbol{\gamma},$$

where \mathbf{X} corresponds to the usual design matrix for the linear effects.

To ensure particular functional forms, prior distributions are assigned to the regression coefficients. The general form of the prior for β_j is

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

where \mathbf{K}_j is a quadratic penalty matrix that shrinks parameters towards zero or penalizes too abrupt jumps between neighboring parameters. In most cases \mathbf{K}_j will be rank deficient and the prior for β_j is partially improper.

The variance parameter τ_j^2 is equivalent to the inverse smoothing parameter in a frequentist approach and controls the trade off between flexibility and smoothness. For full Bayesian inference, weakly informative inverse Gamma hyperpriors $\tau_j^2 \sim IG(a_j, b_j)$ are assigned to τ_j^2 , with $a_j = b_j = 0.001$ as a standard option. Small values for a_j and b_j correspond to an approximate uniform distribution for $\log \tau_j^2$. For empirical Bayes inference, τ_j^2 is considered an unknown constant which is determined via restricted maximum likelihood (REML).

In **BayesX**, estimation of regression parameters is based on three inferential concepts:

1. *Full Bayesian inference via MCMC*

A fully Bayesian interpretation of STAR models is obtained by specifying prior distributions for all unknown parameters. Estimation is carried out using Markov chain Monte Carlo simulation techniques. **BayesX** provides numerically efficient implementations of MCMC schemes for structured additive regression models. Suitable proposal densities have been developed to obtain rapidly mixing, well-behaved sampling schemes without the need for manual tuning ([Brezger and Lang 2006](#)).

2. *Inference via a mixed model representation*

Another concept used for estimation is based on mixed model methodology. The general idea is to take advantage of the close connection between penalty concepts and corresponding random effects distributions. The smoothing variances of the priors then transform to variance components in the random effects (mixed) model. While regression coefficients are estimated based on penalized likelihood, restricted maximum likelihood or marginal likelihood estimation forms the basis for the determination of smoothing parameters. From a Bayesian perspective, this yields empirical Bayes/posterior mode estimates for the STAR models. However, estimates can also merely be interpreted as penalized likelihood estimates from a frequentist perspective ([Fahrmeir et al. 2004](#)).

3. *Penalized likelihood including variable selection*

As a third alternative **BayesX** provides a penalized least squares (or penalized likelihood) approach for estimating STAR models. In addition, a powerful variable and model selection tool is included. Model choice and estimation of the parameters is done simultaneously. The algorithms are able to

- decide whether a particular covariate enters the model,
- decide whether a continuous covariate enters the model linearly or nonlinearly,
- decide whether a spatial effect enters the model,
- decide whether a unit- or cluster-specific heterogeneity effect enters the model

- select complex interaction effects (two dimensional surfaces, varying coefficient terms)
- select the degree of smoothness of nonlinear covariate, spatial or cluster specific heterogeneity effects.

Inference is based on penalized likelihood in combination with fast algorithms for selecting relevant covariates and model terms. Different models are compared via various goodness of fit criteria, e.g. AIC, BIC, GCV and 5 or 10 fold cross validation (Belitz and Lang 2008).

A thorough introduction into the regression models supported by the program is also provided in the **BayesX** methodology manual (Belitz, Brezger, Kneib, and Lang 2011).

4. Implementation in R

The design of the interface attempts to address the following major issues: First, the interfacing function calls should be as practical as possible and oriented on R's standards for regression model fitting functions, second, to provide a set of functions and methods for a convenient representation of fitted model objects, that would enhance the usability of **BayesX**.

In the developing process of package **R2BayesX** we first considered how to connect **BayesX** and R most appropriately. Because **BayesX** does not have an application programming interface (API), amongst others, embedding the sources in an R package seemed to be difficult since the development status of the project is very advanced. The effort of writing and reading data is comparatively small to the processing time needed for estimation of STAR models with **BayesX**. Therefore, we decided to build an interface that primarily sends input program files to the command-line binary version of **BayesX** and reads the returned output files back into R.

We also looked for existing R implementations to get an overview of best practices for software designs including GAM's. The following gives a short summary of some of the larger projects that have added to CRAN. One of the first implementations of GAM's in R is the **gam** package (Hastie and Tibshirani 1990; Hastie 2011). The package is supporting local regression and smoothing splines in combination with a backfitting algorithm and is actually a version of the S-Plus routines for GAM's. The probably best-known and also recommended package is **mgcv** (Wood 2006, 2011a,b), which provides fast and stable algorithms for estimating GAM's based on GCV, REML and others. Vector generalized additive models (VGAM, Yee and Wild 1996) for categorical responses are covered by package **VGAM** (Yee 2010). Another comprehensive package for GAM's, accounting for responses that do not necessarily follow the exponential family and may exhibit heterogeneity, is **gamlss** (Rigby and Stasinopoulos 2005; Stasinopoulos and Rigby 2007). A package based on mixed model technologies is **SemiPar** (Ruppert, Wand, and Carroll 2003; Wand 2010) and its dependent version for adaptive splines **AdaptFit** (Krivobokova 2009). The package **spikeSlabGAM** applies Bayesian variable selection, model choice and regularization for GAMM's (Scheipl 2011).

Within R, regression models are most conveniently specified using its formula language. By reviewing the above mentioned packages for GAM's, we searched for existing structures that on the hand could support a translation method for R commands to **BayesX** interpretable

syntax, and on the other hand, functionality that is already well established, such that applying **R2BayesX** only requires little additional effort for the common R user. Interestingly, most of the packages use different standards for incorporating additive (smooth/special) terms in model formulas and the model frame building process, while a popular name convention for a model term constructor function is “s”, as it is used in package **gam**, **mgcv** and **VGAM**. However, the implementations are again more or less different from each other, i.e. loading packages simultaneously will result in conflicts. The most flexible project seems to be package **mgcv**. Here, similar to package **gam** and **VGAM**, function `s()` does not evaluate design or penalty matrices, but it returns a smooth term definition object of class “**xx.smooth.spec**”, where “**xx**” may be specified by the user. To set up a model with a user defined smooth, a method for the S3 generic function `smooth.construct()`, that returns a design matrix etc., needs to be supplied. Since implementation of additional model terms is also a concern for **R2BayesX** and function `s()` is a quite parsimonious solution, we adopted its functionality and developed methods for a new generic function `bayesx.construct()`, that returns the required command for a particular smooth term in **BayesX**. To give an example, we generate a call to function `s()` with some covariate `x` specifying a P-spline term and return the **BayesX** command with

```
R> bayesx.construct(s(x, bs = "ps"))
```

```
[1] "x(psplinerw2,nrknots=7,degree=4)"
```

Given an R model formula, the specified terms are translated one after another and finally merged into a complete program which may be sent to **BayesX**. Next to the integration of function `s()`, a more **BayesX** alike model term constructor function is provided. The advantage is that a common **BayesX** user may specify models in a more familiar way, which will make a change to **R2BayesX** more easy. The function is called `sx()` and is described in Section 5.4. To avoid package conflicts the new function simply interfaces function `s()`. Moreover, a special constructor function for random effect terms is provided.

The sequence of functions that are consecutively called using the interface is the following: A final program file is generated by first applying function `parse.bayesx.input()` on the R input parameters, including the model formula, data, etc. The returned object is then further processed with function `write.bayesx.input()`, utilizing the methods described above, as well as setting up the necessary data files (folders) to be used with **BayesX**. Afterwards, function `run.bayesx()` executes the program through a call to function `system()`. The output files returned by the binary are imported into R using function `read.bayesx.output()`. Hence, it is also possible to run and read already existing **BayesX** program and output files, see Section 5.5 and the **R2BayesX** manuals for a detailed description. The object returned by function `read.bayesx.output()` is a list of class “**bayesx**”, wherefore a set of base R functions and methods described in Table 3, amongst others, is available. The returned fitted model term objects are also assigned with suitable classes which have plotting methods. Particular effort has been raised on the development of easy to use map effect plots using color legends, see also Section 5.3 and Section 6.

Functions `parse.bayesx.input()`, `write.bayesx.input()`, `run.bayesx()` and `read.bayesx.output()` are combined in the front end main model fitting function `bayesx()` presented in Section 5.3.

5. User interface

5.1. Installing the BayesX binary from R

Before STAR models can be fitted with package **R2BayesX** from R, the binary command-line version of the program **BayesX** needs to be installed and linked to R. The recommended option on UNIX and Windows systems is to auto-compile/install the **BayesX** command-line binary within R by calling the function `install.bayesx()`. Therefore package **R2BayesX** needs to be loaded:

```
R> library("R2BayesX")
```

Installing BayesX from R then ideally only requires running function

```
install.bayesx(inst.dir = NULL, source.dir = NULL, type = NULL)
```

where argument `inst.dir` is a path to a valid installation directory with user writing permissions (e.g. for Windows systems `inst.dir = "C:/BayesX"`). If `source.dir = NULL`, the necessary installation files will automatically tried to be downloaded from the **BayesX** homepage (url: <http://www.stat.uni-muenchen.de/~bayesx>). Otherwise `source.dir` specifies the path where `install.bayesx()` may either find the packed sources `bayesxsource.zip` (url: <http://www.stat.uni-muenchen.de/~bayesx/install/bayesxsource.zip>), or using Windows, the installer `BayesX_windows.exe` (url: http://www.stat.uni-muenchen.de/~bayesx/install/BayesX_windows.exe). If the corresponding file is available, `install.bayesx()` will then attempt to execute the Windows installation process as described in the Appendix A.1, or to compile the sources as shown in Appendix A.2, respectively. If argument `type` is set to `type = "sources"`, compilation of the sources using the GNU Compiler Collection (GCC) C compiler is forced on any platform.

5.2. Linking the BayesX binary to R

After the successful compilation/installation, usually the full path to the command-line binary needs to be declared to R at the beginning of every new session by setting

```
R> options(bayesx.bin = "/path/to/BayesX")
```

where `"/path/to/BayesX"` is e.g. the path provided to argument `inst.dir` of function `install.bayesx()`, with the name of the **BayesX** binary at last. On Windows platforms the name of the binary is `"bayesx.exe"`, on all other platforms commonly `"BayesX"`. Hence, on Windows systems the user may specify e.g.

```
R> options(bayesx.bin = "C:/BayesX/commandline/bayesx.exe")
```

To avoid setting the path to the binary each time R is starting, it is suggested to add the code above to the R startup profile site, see also Appendix A.3. Afterwards, the function call

```
R> check.install.bayesx()
```

will check if **BayesX** is available from R.

5.3. Processing BayesX from R

The main model-fitting function in the package **R2BayesX** is called `bayesx()`. The arguments of `bayesx()` are

```
bayesx(formula, data, weights = NULL, subset = NULL,
       offset = NULL, na.action = na.fail, contrasts = NULL,
       family = "gaussian", method = "MCMC", control = bayesx.control(...),
       ...)
```

where the first two lines basically represent the standard model frame specifications (see [Chambers and Hastie 1992](#)). However, the object supplied to argument `data` is not necessarily an R data object, it is also possible to provide a character string with a path to a dataset stored on disc, which may be reasonable when using large datasets. An example is given in [Section 5.5](#). Additional contrast specifications for factor variables can be passed to argument `contrasts`. Using factors, we recommend deviation or effect coding (see function `contr.sum()`) rather than the usual dummy coding of factors as it typically improves convergence of estimation algorithms used in **BayesX**. The distribution assigned to the response may be set with argument `family`, the default is `family = "gaussian"`. Note that family objects are currently not supported by BayesX. Argument `method` determines the inferential concept used for estimation. Options are: Markov chain Monte Carlo simulation - "MCMC", mixed model based estimation using restricted maximum likelihood/marginal likelihood - "REML" and penalized likelihood including model selection - "STEP". An overview of all available distributions for the different methods is given in [Table 1](#). The last argument specifies several parameters controlling the processing of the **BayesX** binary that are arranged by function `bayesx.control()`. Note that all additional controlling arguments are automatically parsed within function `bayesx()` using the dot dot dot argument "...", which is sent to `bayesx.control()`. The most important parameters for the different methods are listed in [Table 2](#).

The returned fitted model object is a list of class "bayesx", which is supported by several standard extractor functions, such as `plot()` and `summary()`. For models estimated using method "REML", function `summary()` generates summary statistics similar to objects returned from the main model fitting function `gam()` of the **mgcv** package. For "MCMC" estimated models, the mean, standard deviation and quantiles of parameter samples are provided. Using "STEP", the parametric part of the summary statistics is represented like "MCMC", i.e. if computed, the confidence bands are based on an MCMC algorithm subsequent to the model selection, while the remaining summary is similar to "REML". The implemented S3 methods for plotting fitted term objects are quite flexible, i.e., depending on the term structure, the generic function `plot()` calls one of the following functions: for 2d plots function `plot2d()` or `plotblock()` (for factors, unit- or cluster specific plots, draws a block for every estimated parameter including mean and credible intervals), for perspective or image and contour plots function `plot3d()`, map effects plots are produced by function `plotmap()`, with or without colorlegends drawn by function `colorlegend()`, amongst others. See [Table A.4](#) in the Appendix for an overview of the most important arguments for the plotting functions. In some situations it may be useful to inspect the log file generated by the **BayesX** binary.

family	Response distribution	Link	method
"binomial"	binomial	logit	"MCMC" "REML" "STEP"
"binomialprobit"	binomial	probit	"MCMC" "REML" "STEP"
"gamma"	gamma	log	"MCMC" "REML" "STEP"
"gaussian"	Gaussian	identity	"MCMC" "REML" "STEP"
"multinomial"	unordered multinomial	logit	"MCMC" "REML" "STEP"
"poisson"	Poisson	log-link	"MCMC" "REML" "STEP"
"cox"	continuous-time survival data		"MCMC" "REML"
"cumprobit"	cumulative threshold	probit	"MCMC" "REML"
"multistate"	continuous-time multi-state data		"MCMC" "REML"
"binomialcomploglog"	binomial	compl. log-log	"REML"
"cumlogit"	cumulative multinomial	logit	"REML"
"multinomialcatsp"	unordered multinomial (with category-specific covariates)	logit	"REML"
"multinomialprobit"	unordered multinomial	probit	"MCMC"
"seqlogit"	sequential multinomial	logit	"REML"
"seqprobit"	sequential multinomial	probit	"REML"

Table 1: Distributions implemented for methods "MCMC", "REML" and "STEP".

method	Parameter	Description
"MCMC"	iterations	integer, sets the number of iterations for the sampler, default: 12000.
	burnin	integer, sets the burn-in period of the sampler, default: 2000.
	step	integer, defines the thinning parameter for MCMC simulation. E.g., step = 50 means, that only every 50th sampled parameter will be stored and used to compute characteristics of the posterior distribution as means, standard deviations or quantiles, default: 10.
"REML"	eps	numeric, defines the termination criterion of the estimation process. If both the relative changes in the regression coefficients and the variance parameters are less than eps , the estimation process is assumed to have converged, default: 0.00001.
	maxit	integer, defines the maximum number of iterations to be used in estimation. Since the estimation process will not necessarily converge, it may be useful to define an upper bound for the number of iterations.
continued on next page		

continued from previous page	
"STEP"	algorithm character, specifies the selection algorithm. Possible values are "cdescent1" (adaptive algorithms see subsection 6.3 in Belitz et al. 2011), "cdescent2" (adaptive algorithms 1 and 2 with backfitting, see remarks 1 and 2 of section 3 in Belitz and Lang 2008), "cdescent3" (search according to cdescent1 followed by cdescent2 using the selected model in the first step as the start model) and "stepwise" (stepwise algorithm implemented in the <code>gam</code> function of S-plus, see Chambers and Hastie 1992), default: "cdescent1".
	criterion character, specifies the goodness of fit criterion, possible criteria are: "MSEP" (divides the data randomly into a test- and validation dataset. The test dataset is used to estimate the models and the validation dataset is used to estimate the mean squared prediction error (MSEP) which serves as the goodness of fit criterion to compare different models), "GCV" (Generalized Cross Validation based on deviance residuals, see e.g. Wood 2006), "GCVrss" (Generalized Cross Validation based on residual sum of squares, see e.g. Wood 2006), "AIC" (Akaike Information Criterion, see e.g. Burnham and Anderson 1998), "AIC_imp" (improved AIC with bias correction for regression models, see e.g. Burnham and Anderson 1998), "BIC" (Bayesian information criterion, see e.g. Hastie, Tibshirani, and Friedman 2009), "MSEP", "CV5" (5-fold cross validation, see e.g. Hastie et al. 2009), "CV10" (5-fold cross validation, see e.g. Hastie et al. 2009) and "AUC" (area under the ROC curve, binary response only), default: "AIC_imp".
	startmodel character, defines the start model for variable selection. Options are "linear" (start model with degrees of freedom equal to one for model terms), "empty" (empty model containing only an intercept), "full" (most complex possible model) and "userdefined" (start model is specified by the user), default: "linear".

Table 2: Most important controlling parameters for the different methods using function `bayesx()`. (A detailed documentation is provided in the manual of function `bayesx.control()` of package **R2BayesX**.)

The file can either be viewed directly during processing if argument `verbose` is set to `TRUE` in function `bayesx.control()`, or extracted from the fitted model object using function `bayesx_logfile()`. For MCMC post estimation diagnosis, besides the implemented trace and autocorrelation plots, samples of the parameters may also be extracted using function `samples()`. The sampling paths are provided as a data frame, and hence may e.g. be converted to objects of class "mcmc" using the **coda** package ([Plummer, Best, Cowles, and Vines 2006](#)) for further analysis. In addition, an R script for the estimated model, including func-

Function	Description
<code>print()</code>	simple printed display of the initial call and some additional information of the fitted model.
<code>summary()</code>	returns an object of class <code>"summary.bayesx"</code> containing the relevant summary statistics (which has a <code>print()</code> method).
<code>coef()</code>	extracts coefficients of the linear modeled terms.
<code>confint()</code>	compute confidence intervals of linear modeled terms if <code>method = "REML"</code> , for <code>"MCMC"</code> the quantiles of the coefficient samples according to a specified probability level are computed.
<code>cprob()</code>	extract contour probabilities of a particular P-spline term, only meaningful if <code>method = "MCMC"</code> and argument <code>contourprob</code> is specified as an additional argument in the term constructor function <code>sx()</code> , or within argument <code>xt</code> in function <code>s()</code> . E.g. in the introductory example, contour probabilities for the term using covariate <code>mbmi</code> are estimated with <code>s(mbmi, bs = "ps", xt = list(contourprob = 4))</code> (see also Section 5.4).
<code>fitted()</code>	fitted values of either the mean and linear predictor, or a selected model term.
<code>bayesx_logfile()</code> , <code>bayesx_prgrfile()</code> , <code>bayesx_runtime()</code>	extracts the internal BayesX log file, the program file and the overall runtime of the binary.
<code>residuals()</code>	extract model or partial residuals for a selected term.
<code>samples()</code>	extract samples of parameters from MCMC simulation.
<code>terms()</code>	extract terms of model components.
<code>model.frame()</code>	extract/generate a model frame.
<code>logLik()</code>	extract fitted log-likelihood, only if <code>method = "REML"</code> .
<code>plot()</code>	either model diagnostic plots or effect plots of particular terms.
<code>getscript()</code>	generate an R script for term effect, diagnostic plots and model summary statistics.
<code>AIC()</code> , <code>BIC()</code> , <code>DIC()</code> , <code>GCV()</code>	computes information criteria, availability is dependent on the <code>method</code> used.

Table 3: Functions and methods for objects of class `"bayesx"`. (A detailed documentation is provided in the manual of package **R2BayesX**.)

tion calls for saving, loading, plotting of term effects and diagnostic plots, may be generated using function `getscript()`. The produced R script may be useful for less experienced users of the package to get a quick overview of post estimation commands. Moreover, the script facilitates the final preparation of plots and diagnostics to be included in publications. A list of all available functions and methods of package **R2BayesX** can be found in Table 3.

5.4. Available additive terms

In package **R2BayesX**, the main constructor function for specifying additive terms in STAR formulas is called `sx()`. The function is basically an interface to the term constructor function `s()` of package **mgcv**, also see Section 4.

The arguments of function `sx()` are

```
sx(x, z = NULL, bs = "ps", by = NA, ...)
```

where `x` represents the covariate that is used for univariate and `z` for bivariate model terms. Argument `bs` chooses the basis/type of the term, possible options are shown in Table 4.

Note that it is possible to specify all term type versions presented in the table, the short and the original ones that are used within **BayesX**, e.g. `bs = "ps"` or `bs = "psplinerw2"` result in the same type of model term. A numeric or a factor variable can be provided to argument `by` to estimate varying coefficient terms, where the effect of the variable provided to `by` varies over the range of the covariate(s) of this term. The dot dot dot “...” argument is used to specify term specific control parameters or additional geographical information. In the example Section 2, to modify the degree and the inner knots for the P-spline term `sx(mbmi)`, the user may e.g. type `sx(mbmi, degree = 2, knots = 10)`. For supplying additional boundary or graph files (see function `read.bnd()`, `read.gra()`, `shp2bnd()` and `bnd2gra()` for importing and creation of spatial objects that may be sent to **BayesX**), that are used to compute suitable neighborhood penalty matrices for terms using Markov random field priors, or to calculate the centroids of particular regions for geosplines and geokriging terms, an argument named `map` needs to be provided. For instance, the necessary boundary file `ZambiaBnd` for the geokriging term in Section 2 is included with `sx(district, bs = "gk", map = ZambiaBnd)`. Information about all possible extra arguments for a particular term basis/type can be looked up using function `bayesx.term.options()`, e.g. possible options for P-splines using “MCMC” are printed to the console by

```
R> bayesx.term.options(bs = "ps", method = "MCMC")
```

```
possible options for 'bs = "ps"':
```

```
degree: the degree of the B-spline basis functions.
```

```
Default: integer, 'degree = 3'.
```

```
knots: number of inner knots.
```

```
Default: integer, 'knots = 20'.
```

For reasons of simplicity only the first two additional controlling arguments are shown.

Some care has to be taken with the identifiability of varying coefficients terms. The standard in **BayesX** is to center nonlinear main effects terms around zero whereas varying coefficient terms are not centered. This makes sense since main effects nonlinear terms are not identifiable and varying coefficients terms are usually identifiable. However, there are situations where a varying coefficients term is not identifiable. Then the term must be centered. Since centering is not automatically accomplished it has to be enforced by the user by adding option `center = TRUE` in function `sx()`. To give an example, the varying coefficient terms in $\eta = \dots + g_1(z_1)z + g_2(z_2)z + \gamma_0 + \gamma_1 z + \dots$ are not identified, whereas in $\eta = \dots + g_1(z_1)z + \gamma_0 + \dots$, the varying coefficient term is identifiable. In the first case, centering is necessary, in the second case, it is not.

bs	Description
"rw1", "rw2"	zero degree P-splines: defines a zero degree P-spline with first or second order difference penalty. A zero degree P-spline typically estimates for every distinct covariate value in the dataset a separate parameter. Usually there is no reason to prefer zero degree P-splines over higher order P-splines. An exception are ordinal covariates or continuous covariates with only a small number of different values. For ordinal covariates higher order P-splines are not meaningful while zero degree P-splines might be an alternative to modeling nonlinear relationships via a dummy approach with completely unrestricted regression parameters.
"season"	seasonal effect of a time scale.
"ps", "psplinerw1", "psplinerw2"	P-spline with first or second order difference penalty.
"te", "pspline2dimrw1"	defines a two-dimensional P-spline based on the tensor product of one-dimensional P-splines with a two-dimensional first order random walk penalty for the parameters of the spline.
"kr", "kriging"	kriging with stationary Gaussian random fields.
"gk", "geokriging"	geokriging with stationary Gaussian random fields: estimates a stationary Gaussian random field based on the centroids of a map object provided in boundary format (see function <code>read.bnd()</code> and <code>shp2bnd()</code>) as an additional argument named <code>map</code> within function <code>sx()</code> , or supplied within argument <code>xt</code> when using function <code>s()</code> , e.g. <code>xt = list(map = MapBnd)</code> .
"gs", "geospline"	geosplines based on two-dimensional P-splines with first order random walk penalty: defines a two-dimensional P-spline for the spatial covariate region with a two-dimensional first order random walk penalty for the parameters of the spline. Estimation is based on the coordinates of the centroids of the regions of a map object provided in boundary format (see function <code>read.bnd()</code> and <code>shp2bnd()</code>) as an additional argument named <code>map</code> within function <code>sx()</code> , or supplied within argument <code>xt</code> when using function <code>s()</code> , e.g. <code>xt = list(map = MapBnd)</code> .
"mrf", "spatial"	Markov random fields: defines a Markov random field prior for a spatial covariate, where geographical information is provided by a map object in boundary or graph file format (see function <code>read.bnd()</code> , <code>read.gra()</code> and <code>shp2bnd()</code>), as an additional argument named <code>map</code> within function <code>sx()</code> , or supplied within argument <code>xt</code> when using function <code>s()</code> , e.g. <code>xt = list(map = MapBndorGra)</code> .
continued on next page	

continued from previous page	
"bl", "baseline"	nonlinear baseline effect in hazard regression or multi-state models: defines a P-spline with second order random walk penalty for the parameters of the spline for the log-baseline effect $\log(\lambda(\text{time}))$.
"factor"	special BayesX specifier for factors, especially meaningful if <code>method = "STEP"</code> , since the factor term is then treated as a full term, which is either included or removed from the model.
"ridge", "lasso", "nigmix"	shrinkage of fixed effects: defines a shrinkage-prior for the corresponding parameters γ_j , $j = 1, \dots, q$, $q \geq 1$ of the linear effects x_1, \dots, x_q . There are three priors possible: ridge-, lasso- and Normal Mixture of inverse Gamma prior.

Table 4: Possible **BayesX** model terms within function `sx()` and `s()`.

As mentioned above, users may optionally call the constructor function `s()` directly. The usage of `s()` in **R2BayesX** is in principle similar to package **mgcv**. The applicable arguments are

```
s(..., k = -1, bs = "ps", m = NA, by = NA, xt = NULL)
```

Within `s()`, the list of covariates used for the model term is set with argument "...". For instance, in the example of Section 2, the term for the body mass index of the mother may also be included in the model formula by `s(mbmi)`, a term with two covariates is specified e.g. with `s(mbmi, agechild)`. Here, the parameter `k` controls the dimension of the basis used for smooth terms. Setting argument `m` is only meaningful for P-splines, i.e. `bs = "ps"`, and controls the degree of the B-spline basis functions and the order of the difference penalty. E.g. a B-spline of degree 3 with a 2nd order difference penalty is set with `s(mbmi, bs = "ps", m = c(1, 2))` (note that argument `m` is slightly different than argument `degree` in function `sx()` using P-splines, see also the manual of `s()`). Argument `by` is used in the same way as for `sx()`. The additional parameters that are specified by argument "..." in function `sx()`, may be set in `s()` within argument `xt`, e.g. similar to the example above, the boundary object `ZambiaBnd` is supplied with `s(district, bs = "gk", xt = list(map = ZambiaBnd))`. Besides `s()`, **R2BayesX** also supports calls to the tensor product constructor function `te()`, however, only a small set of the features of this function is supported.

In addition to `sx()`, `s()` and `te()`, unit- or cluster specific unstructured (random) effects may be incorporated into the model formula using the random effects term constructor function `r()`. The arguments of `r()` are

```
r(id, by = NA, xt = NULL)
```

where `id` is the unit or cluster identification covariate the random effects should be estimated for. E.g. the model formula from the introduction could be extended by a random effects term for the districts in Zambia with `r(district)`. Argument `by` takes covariates for which random slopes may be estimated. Argument `xt` is used in the same way as described for function `s()`, i.e. similar to the above, e.g. hyperpriors a and b for the variance parameter are set with `r(district, xt = list(a = 0.0001, b = 0.0001))`.

5.5. Additional options

For most practical purposes fitting models with function `bayesx()` may be sufficient. However, the interfacing functions that are consecutively called within `bayesx()` can also be used independently. This could be meaningful for two reasons: First, users may want to use already existing **BayesX** program files wherefore a new setup within R is not required, and secondly, there might be a need for automated importing of **BayesX** output files into R for further analysis.

Function `run.bayesx()` is used to run an arbitrary **BayesX** program file. The arguments of `run.bayesx()` are

```
run.bayesx(dir, prg.name = "bayesx.estim.input.prg",
  verbose = TRUE, bin = getOption("bayesx.bin"))
```

where `dir` is a character string with the directory the program file is stored in and `prg.name` is the name of the corresponding program file. During processing of **BayesX** several informations will be printed to the R console if `verbose = TRUE`. Argument `bin` specifies the location of the **BayesX** binary the program file is sent to, see also Section 5.2. The function returns a list including the log file returned by **BayesX** as well as information on the total runtime.

Model output files are imported using function

```
read.bayesx.output(dir, model.name = NULL)
```

Here, `dir` is again a directory and `model.name` the name of the model the files are imported for, also provided as character strings. Note that the function will search for all different BayesX estimated models in the declared directory if argument `model.name` is set to `NULL`. The returned object is also of class "bayesx", i.e. all the functions and methods described in Table 3 may be applied.

Another noteworthy feature of package **R2BayesX** is the internal handling of data. **BayesX** uses numerically efficient algorithms including sparse matrix computations which in principle allow to estimate models using large datasets. Moreover, the number of different observations for particular covariates is usually much smaller than the total number of observations. That is, the output files returned by the binary only include estimates for unique covariate values. Since these files typically reserve much less disc space, importing the fitted model objects into R using `read.bayesx.output()` is straightforward in most cases, whereas handling the complete dataset within R may be problematic. As mentioned in Section 5.3, users can exploit this by providing a character string to argument `data` in function `bayesx()`, which includes the path to a dataset instead of an R data object. As a consequence, this dataset will not be loaded within R and is only used internally by the **BayesX** binary. To give an example, we generate a large dataset that might produce problems with R's memory allocation using a model fitting function, especially if the model contains a large number of parameters. Therefore, we store the data on disc in the temporary folder of the running session with

```
R> set.seed(321)
R> file <- paste(tempdir(), "/data.raw", sep = "")
R> n <- 5e+06
R> dat <- data.frame(x = rep(runif(1000, -3, 3), length.out = n))
```

```
R> dat$y <- with(dat, sin(x) + rnorm(n, sd = 2))
R> write.table(dat, file = file, quote = FALSE, row.names = FALSE)
```

This produces a dataset of approximately 170Mb with only 1000 unique observations for covariate x . The path to the dataset is stored in object `file` and is provided to argument `data` in the function call

```
R> b <- bayesx(y ~ sx(x), family = "gaussian", method = "MCMC",
+   iterations = 3000, burnin = 1000, step = 2, predict = FALSE,
+   data = file, seed = 123)
```

For illustration purposes, the number of iterations is only set to 3000. Note that argument `predict` is set to `FALSE`, i.e. only output files of estimated effects will be returned, otherwise an expanded dataset using all observations would be written in the output directory, also containing the data used for estimation. The runtime of this example is about 4 1/2 hours

```
R> bayesx_runtime(b)

      user   system elapsed
16442.12    7.56 16461.33
```

on a Linux system with an Intel 2.33GHz Dual Core processor, while the returned object `b` uses

```
R> print(object.size(b), units = "Mb")
```

```
0.4 Mb
```

of memory size.

6. STAR models in practice

The focus of this section is on demonstrating the various features of the **R2BayesX** package. Therefore, the examples provided are replicate analysis taken from [Brezger *et al.* \(2005\)](#) and [Fahrmeir *et al.* \(2009\)](#). The presented datasets have been added to package **R2BayesX**, ensuring straightforward traceability of the following code. In the first example, a Gaussian regression model is estimated using Markov chain Monte Carlo simulation. The second example covers estimation based on mixed model technology, where a cumulative threshold model is assigned for the response variable (see [Fahrmeir and Tutz \(2001\)](#) and [Kneib and Fahrmeir \(2004\)](#) for cumulative threshold models). The last example illustrates the approach of the stepwise algorithm for model and variable selection.

6.1. Childhood malnutrition in Zambia: Analysis with MCMC

This analysis has already been conducted by [Kandala *et al.* \(2001\)](#) and has also been used as a demonstrating example in [Brezger *et al.* \(2005\)](#). Stunting is one of the leading drivers of a number of problems development countries are faced with, for instance, a direct consequence

of stunting is a high mortality rate. Here, the primary interest is to model the dependence of stunting of newborn children, with an age ranging from 0 to 5 years, on covariates such as the body mass index of the mother, the age of the child and others presented in Table 5. The response `stunting` is standardized in terms of a reference population, i.e. in this dataset

Variable	Description
<code>stunting</code>	standardized Z-score for stunting.
<code>mbmi</code>	body mass index of the mother.
<code>agechild</code>	age of the child in months.
<code>district</code>	district where the mother lives.
<code>memployment</code>	mother's employment status with categories 'yes' and 'no'.
<code>meducation</code>	mother's educational status with categories for no education or incomplete primary 'no', complete primary but incomplete secondary 'primary' and complete secondary or higher 'secondary'.
<code>urban</code>	locality of the domicile with categories 'yes' and 'no'.
<code>gender</code>	gender of the child with categories 'male' and 'female'.

Table 5: Variables in the dataset on childhood malnutrition in Zambia.

stunting for child i is represented by

$$\text{stunting}_i = \frac{AI_i - MAI}{\sigma},$$

where AI refers to a child's anthropometric indicator (height at a certain age in our example), while MAI and σ correspond to the median and the standard deviation in the reference population, respectively.

Following [Kandala *et al.* \(2001\)](#), we estimate a structured additive regression model with predictor

$$\begin{aligned} \eta = & \gamma_0 + \gamma_1 \text{memploymentyes} + \gamma_2 \text{urbanno} + \gamma_3 \text{genderfemale} + \\ & \gamma_4 \text{meducationno} + \gamma_5 \text{meducationprimary} + \\ & f_1(\text{mbmi}) + f_2(\text{agechild}) + f_{str}(\text{district}) + f_{unstr}(\text{district}) \end{aligned} \quad (2)$$

where `memploymentyes` is the deviation (effect) coded version of covariate `memployment`, generated with function `contr.sum()` by setting the contrasts argument of the factor variable, i.e. `memploymentyes` contains of values -1, corresponding to 'yes', and 1, 'no' respectively, likewise for covariates `genderfemale`, `urbanno`, `meducationno` and `meducationprimary`. As mentioned in the introduction, functions f_1 and f_2 of the continuous covariates `agechild` and `mbmi` are assumed to have a possibly nonlinear effect on `stunting` and are therefore modeled with P-splines. Furthermore, the spatial effect is decomposed into a structured effect f_{str} , modeled by a Gaussian Markov random field, and an unstructured effect f_{unstr} , using a random effects term for the districts in Zambia.

The data for this analysis is provided in the **R2BayesX** package and can be loaded with

```
R> data("ZambiaNutrition", package = "R2BayesX")
```

Since function f_{str} is modeled by a Markov random fields term, **BayesX** needs information about the district neighborhood structure, which e.g. is enclosed in the file

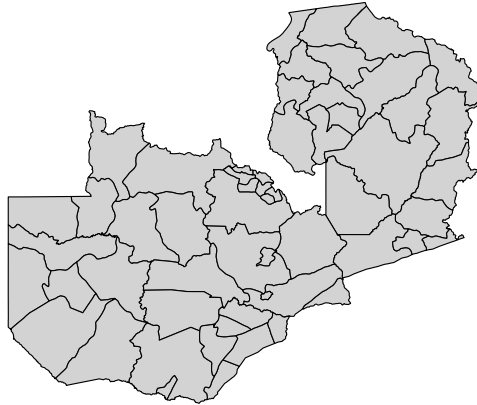


Figure 2: Example on childhood malnutrition: A simple map of the districts in Zambia.

```
R> data("ZambiaBnd", package = "R2BayesX")
```

The object `ZambiaBnd` has class `"bnd"` and is basically a `list()` of polygon matrices, with x - and y -coordinates of the boundary points in the first and second column respectively. To read in an arbitrary boundary file into R function `read.bnd()` can be used. With the information of the boundary file **BayesX** may compute an appropriate adjacency matrix, allowing for a smoothly varying effect of the neighboring regions. There is a generic plotting method implemented for objects of class `"bnd"`, which in principle calls function `plotmap()`. E.g. a simple map, as shown in Figure 2, of the districts in Zambia is drawn by typing

```
R> plot(ZambiaBnd)
```

Having loaded the necessary files, the model formula is specified with

```
R> f <- stunting ~ memployment + urban + gender + meducation +
+   sx(mbmi) + sx(agechild) + sx(district, bs = "mrf", map = ZambiaBnd) +
+   r(district)
```

The model is then fitted using MCMC by calling

```
R> zm <- bayesx(f, family = "gaussian", method = "MCMC",
+   iterations = 12000, burnin = 2000, step = 10,
+   seed = 123, data = ZambiaNutrition)
```

Argument `iterations`, `burnin` and `step` set the number of iterations of the MCMC simulation, the burnin period, which will be removed from the generated samples, and the step length for which samples should be stored, i.e. if `step = 10`, every 10th sampled parameter will be saved. In most applications 12000 iterations should be enough for a valid fit with sufficiently small autocorrelations of stored parameters, at least in the model building stage. However, it is absolutely necessary to take a look at sampled parameters and autocorrelation functions to check the mixing behavior (see below). Moreover, it is generally advisable to specify a higher number of iterations for the final model that appears in publications. Argument `seed` sets the state of the random number generator in **BayesX**, which is meaningful for exact replication of the examples.

After the model has been successfully fitted, summary statistics of the MCMC estimated model object may be printed with

```
R> summary(zm)
```

Call:

```
bayesx(formula = f, data = ZambiaNutrition, family = "gaussian",
        method = "MCMC", iterations = 12000, burnin = 2000, step = 10,
        seed = 123)
```

Fixed effects estimation results:

Parametric Coefficients:

	Mean	Sd	2.5%	50%	97.5%
(Intercept)	0.1013	0.0479	0.0076	0.1024	0.1927
memploymentyes	-0.0076	0.0139	-0.0356	-0.0072	0.0206
urbanno	-0.0900	0.0221	-0.1343	-0.0896	-0.0477
genderfemale	0.0583	0.0129	0.0338	0.0584	0.0833
meducationno	-0.1736	0.0277	-0.2256	-0.1731	-0.1203
meducationprimary	-0.0616	0.0255	-0.1126	-0.0624	-0.0130

Smooth terms variances:

	Mean	Sd	2.5%	50%	97.5%	Min	Max
sx(agechild)	0.0059	0.0057	0.0012	0.0042	0.0192	0.0005	0.0699
sx(district)	0.0356	0.0185	0.0101	0.0320	0.0824	0.0035	0.1317
sx(mbmi)	0.0018	0.0024	0.0003	0.0011	0.0078	0.0002	0.0307

Random effects variances:

	Mean	Sd	2.5%	50%	97.5%	Min	Max
r(district)	0.0073	0.0059	0.0006	0.0056	0.0215	0.0002	0.0374

Scale estimate:

	Mean	Sd	2.5%	50%	97.5%
Sigma2	0.8018	0.0165	0.7718	0.8017	0.8342

```
N = 4847 burnin = 2000 DIC = 4903.618 pd = 50.48634
method = MCMC family = gaussian iterations = 12000 step = 10
```

which typically includes mean, standard deviation and quantiles of sampled linear effects, smooth terms variances and random effects variances, as well as goodness of fit criteria and some other information about the model. The estimated effects for covariates `agechild` and `mbmi` may then be visualized with

```
R> plot(zm, term = c("sx(mbmi)", "sx(agechild)"))
```

and are shown in Figure 3.

A visual representation of the structured and unstructured spatial effect can be obtained in two ways. Using the plain plot function

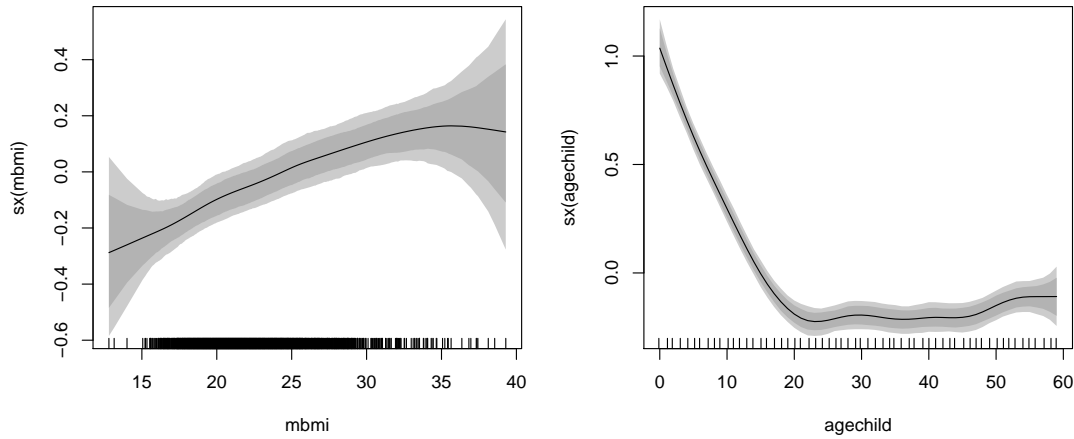


Figure 3: Example on childhood malnutrition: Effect of the body mass index of the child's mother and of the age of the child together with pointwise 80% and 95% credible intervals.

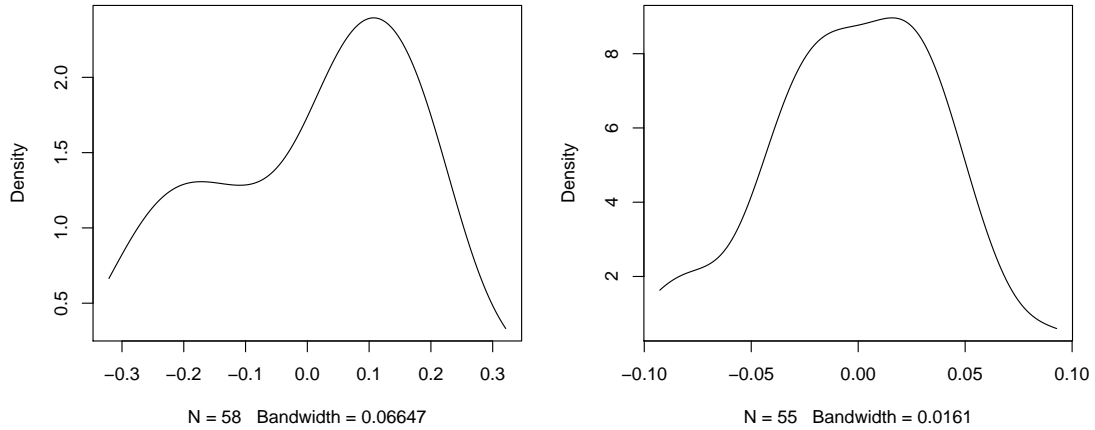


Figure 4: Example on childhood malnutrition: Kernel density estimates of the mean of the structured, left panel, and the unstructured spatial effect, right panel respectively.

```
R> plot(zm, term = c("sx(district)", "r(district)"))
```

produces a kernel density estimator of the posterior mean of the effects, see Figure 4. The kernel densities reveal the general form of the random effects distributions. To view the spatial structure of the correlated effect we have to use the plot function in combination with the boundary object `ZambiaBnd`:

```
R> plot(zm, term = "sx(district)", map = ZambiaBnd)
```

The generated map effect plot is shown in Figure 5. As a default the districts of Zambia are colored in a symmetrical range within $+\max(|\min(pmean)|, |\max(pmean)|)$. In many situations the visual impression of the colored map is problematic. This is primarily the case if there are some districts with extraordinarily high posterior means compared to the rest of the districts. Then the map is dominated by the colors of these outlying districts. A more informative map may be obtained by restricting the range of the plotting area using

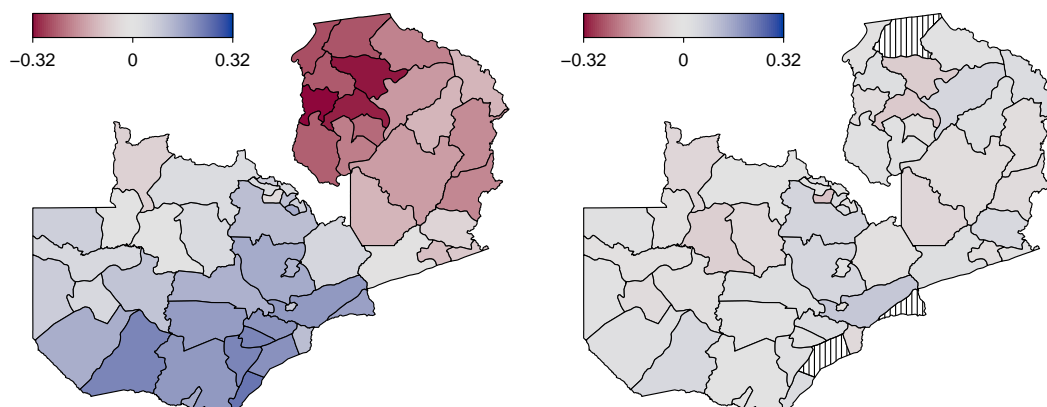


Figure 5: Example on childhood malnutrition: Estimated mean effect of the structured spatial effect (left panel), together with the unstructured spatial effect using the color and legend scaling of the structured effect (right panel).

the range option. For the Zambia data the corresponding random effects are comparably symmetric and without outlying districts such that the plot function with default options produces fairly informative maps. To demonstrate the range option we draw the unstructured random effect and the legend range within the same range as the structured random effect

```
R> range <- lrange <- c(-0.32, 0.32)
R> plot(zm, term = "r(district)", map = ZambiaBnd,
+       range = range, lrange = lrange)
```

The resulting map is also shown in Figure 5 (right panel). Using for both the structured and the unstructured effect the same scale is useful for comparison. In most cases one of the two effects clearly dominates the other. In our case the structured spatially correlated effect clearly exceeds the unstructured effect.

For MCMC post estimation diagnosis, it is also possible to extract sampling paths of parameters with function `samples()`, or to plot the samples directly. For instance, coefficient sampling paths for term `sx(mbmi)` are displayed with

```
R> plot(zm, term = "sx(mbmi)", which = "coef-samples")
```

see Figure 6. The plot of sampled parameters should ideally show white noise, i.e. more or less uncorrelated samples that show no particular pattern. In our case the samples are exactly as they should be. In addition, autocorrelation functions may be drawn, e.g. for the variance samples of term `sx(mbmi)`, by typing

```
R> plot(zm, term = "sx(mbmi)", which = "var-samples", acf = TRUE)
```

The maximum autocorrelation of all sampled parameters in the model are displayed with

```
R> plot(zm, which = "max-acf", acf = TRUE)
```

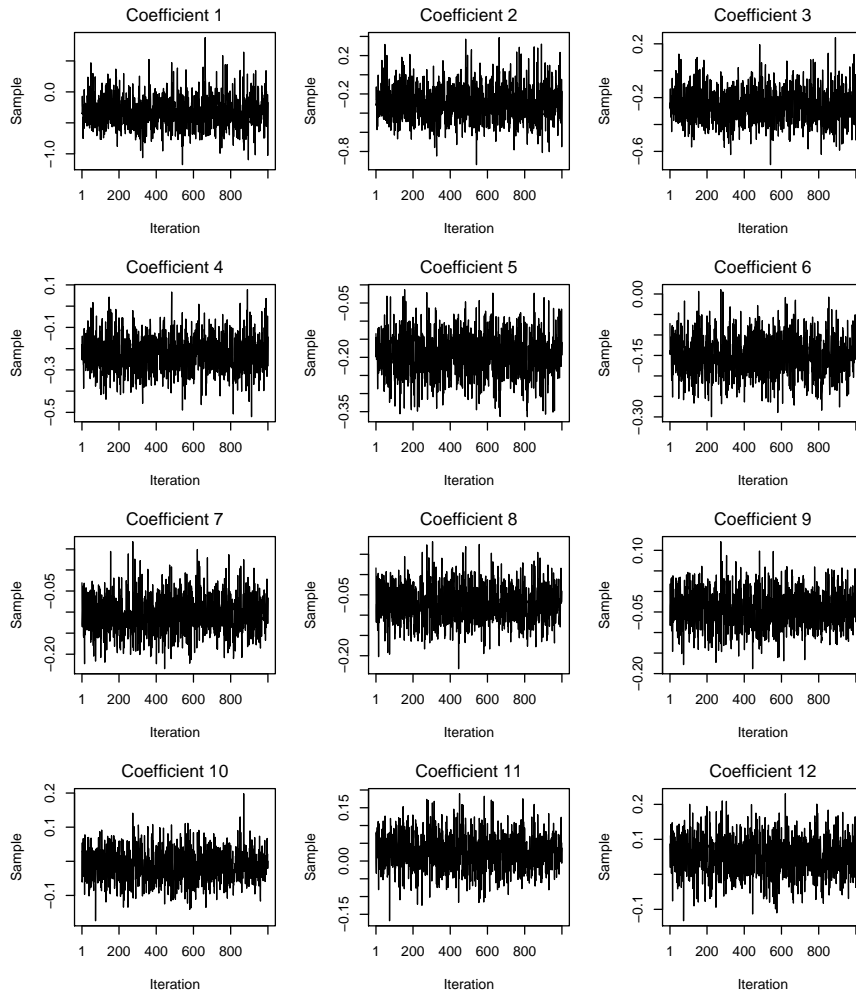


Figure 6: Example on childhood malnutrition: Sampling paths of the first 12 coefficients of term `sx(mbmi)`.

Autocorrelations for all lags should be close to zero as is mostly the case in our example. See Figure 7, for the autocorrelation plots. The plot of maximum autocorrelations over all model parameters suggests to use a larger number of iterations in a final run (e.g. 22000 or even 32000 iterations).

In some situations problems may occur during processing of the **BayesX** binary, that are not automatically detected by the main model fitting function `bayesx()`. Therefore the user may inspect the log-file generated by the binary in two ways: Setting the option `verbose = TRUE` in `bayesx.control()` will print all information produced by **BayesX** simultaneously at runtime. The option is especially helpful if **BayesX** crashes. Another way to obtain the log-file is to use function `bayesx_logfile()` if **BayesX** successfully finished processing. In this example the log-file may be printed with

```
R> bayesx_logfile(zm)
```

```
> bayesreg b
```

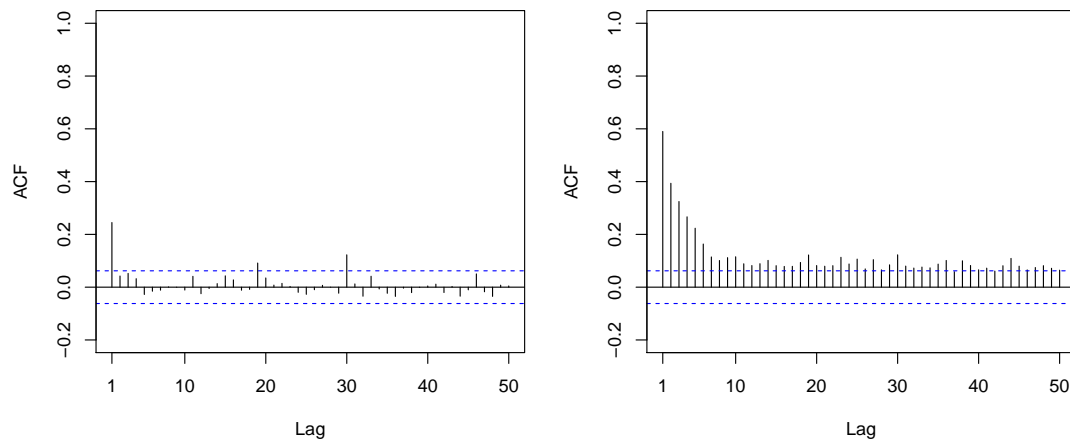


Figure 7: Example on childhood malnutrition: Autocorrelation function of the samples of the variance parameter of term `sx(mbmi)`, left panel, maximum autocorrelation of all parameters of the model, right panel respectively.

```
> map ZambiaBnd
> ZambiaBnd.infile using /tmp/Rtmpa3Z6WF/bayesx/ZambiaBnd.bnd
NOTE: 57 regions read from file /tmp/Rtmpa3Z6WF/bayesx/ZambiaBnd.bnd
> dataset d
> d.infile using /tmp/Rtmpa3Z6WF/bayesx/bayesx.estim.data.raw
NOTE: 14 variables with 4847 observations read from file
/tmp/Rtmpa3Z6WF/bayesx/bayesx.estim.data.raw

> b.outfile = /tmp/Rtmpa3Z6WF/bayesx/bayesx.estim
> b.regress stunting = mbmi(psplinerw2,nrknots=20,degree=3) +
  agechild(psplinerw2,nrknots=20,degree=3) + district(spatial,map=ZambiaBnd) +
  district(random) + memploymentyes + urbanno + genderfemale + mededucationno +
  mededucationprimary, family=gaussian iterations=12000 burnin=2000 step=10
  setseed=123 predict using d
NOTE: no observations for region 11
NOTE: no observations for region 84
NOTE: no observations for region 96
```

BAYESREG OBJECT b: regression procedure

GENERAL OPTIONS:

```
Number of iterations: 12000
Burn-in period:      2000
Thinning parameter:  10
```

RESPONSE DISTRIBUTION:

```

Family: Gaussian
Number of observations: 4847
Number of observations with positive weights: 4847
Response function: identity
Hyperparameter a: 0.001
Hyperparameter b: 0.001

```

To simplify matters only a fragment of the log-file is shown in the above. The log-file typically provides information on the used data, model specifications, algorithms and possible error messages.

6.2. Forest health dataset: Analysis with REML

The dataset on forest health comprises information on the defoliation of beech trees, which serves as an indicator of overall forest health here. The data was collected annually from 1980 to 1997 during a project of visual inspection of trees around Rothenbuch, Germany, see [Göttlein and Pruscha \(1996\)](#), and is discussed in detail in [Fahrmeir *et al.* \(2009\)](#). In this example, the percentage rate of defoliation of each tree is aggregated into three ordinal categories, which are modeled in terms of covariates characterizing the stand and site of a tree. In addition, temporal and spatial information is available, see also [Table 6](#).

Variable	Description
id	tree location identification number.
year	year of census.
defoliation	percentage of tree defoliation in three ordinal categories, ‘defoliation < 12.5%’, ‘12.5% ≤ defoliation < 50%’ and ‘defoliation ≥ 50%’.
age	age of stands in years.
canopy	forest canopy density in percent.
inclination	slope inclination in percent.
elevation	elevation (meters above sea level).
soil	soil layer depth in cm.
ph	soil pH at 0-2cm depth.
moisture	soil moisture level with categories ‘moderately dry’, ‘moderately moist’ and ‘moist or temporarily wet’.
alkali	proportion of base alkali-ions with categories ‘very low’, ‘low’, ‘high’ and ‘very high’.
humus	humus layer thickness in cm.
stand	stand type with categories ‘deciduous’ and ‘mixed’.
fertilized	fertilization applied with categories ‘yes’ and ‘no’.

Table 6: Variables in the forest health dataset.

Similar to [Fahrmeir *et al.* \(2009\)](#), we start with a threshold model and cumulative logit link, with $P(\text{defoliation}_{it} \leq r)$ of tree i at time t , $r = 1, 2$, and the additive predictor

$$\eta_{it}^{(r)} = f_1(\text{age}_{it}) + f_2(\text{inclination}_i) + f_3(\text{canopy}_{it}) + f_4(\text{year}) + f_5(\text{elevation}_i) + \mathbf{x}_{it}'\boldsymbol{\gamma}$$

where f_1, \dots, f_5 are possibly nonlinear smooth functions of the continuous covariates and $\mathbf{x}'_{it}\boldsymbol{\gamma}$ comprises covariates with parametric effects using deviation (effect) coding for factor covariates.

To estimate the model within R the data is loaded and the model formula specified with

```
R> data("ForestHealth", package = "R2BayesX")
R> f <- defoliation ~ stand + fertilized +
+   humus + moisture + alkali + ph + soil +
+   sx(age) + sx(inclination) + sx(canopy) +
+   sx(year) + sx(elevation)
```

The covariates entering nonlinearly are again modeled by P-splines. The model is then fitted applying REML by assigning a cumulative logit model and calling

```
R> fm1 <- bayesx(f, family = "cumlogit",
+   method = "REML", data = ForestHealth)
```

After the estimation process has converged, the estimated effects of the nonparametric modeled terms may be visualized by typing

```
R> plot(fm1, term = c("sx(age)", "sx(inclination)",
+   "sx(canopy)", "sx(year)", "sx(elevation)"))
```

and are shown in Figure 8. In this example some contradictory results occur. The effect of covariate **age** on the **defoliation** seems to decline for both, younger and older trees, which intuitively should be a monotone increasing effect, this also holds for the effect of **elevation**. Moreover, the extremely wiggly estimate of **inclination** is hardly interpretable. Therefore, [Göttlein and Pruscha \(1996\)](#) extend the model by a spatial effect, which is modeled by a two dimensional geospline term of the tree locations. The tree x - and y -coordinates are calculated by the centroid positions of tree polygons given by the boundary map file, which may be loaded with

```
R> data("BeechBnd", package = "R2BayesX")
```

We now fit the model:

```
R> f <- update(f, ~ . + sx(id, bs = "gs", map = BeechBnd))
R> fm2 <- bayesx(f, family = "cumlogit",
+   method = "REML", data = ForestHealth)
```

Taking a look at model information criteria with

```
R> BIC(fm1, fm2)
```

	df	BIC
fm1	59.9714	2016.04
fm2	94.8222	1930.06

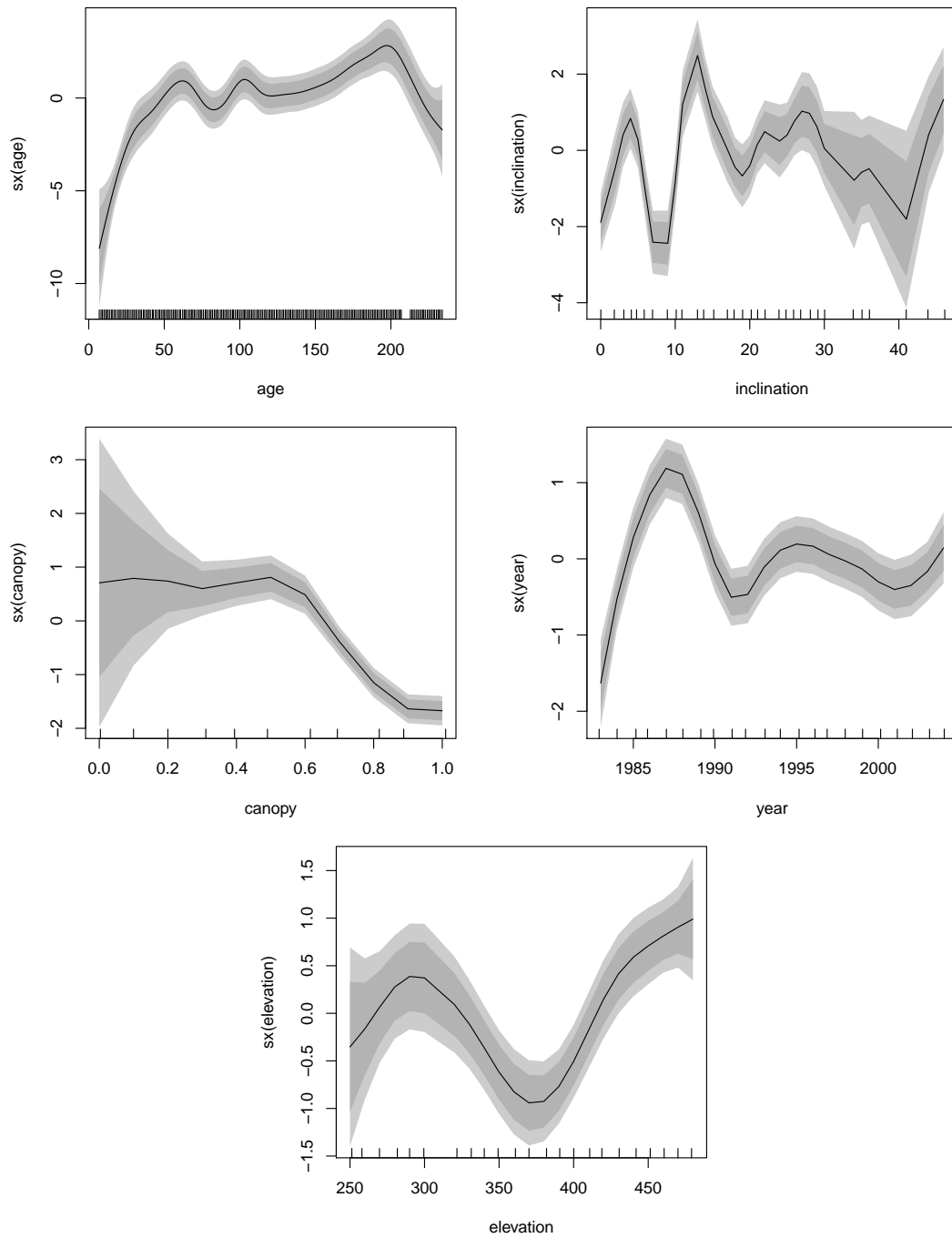


Figure 8: Forest damage: Estimates of nonparametric effects including 80% and 95% point-wise confidence intervals of the model without the spatial effect.

```
R> GCV(fm1, fm2)
```

	df	GCV
fm1	59.9714	0.816340
fm2	94.8222	0.610199

clearly indicates a better fit by modeling the spatial effect of tree locations. The summary statistics for both models gives:

```
R> summary(fm1)
```

Call:

```
bayesx(formula = f, data = ForestHealth, family = "cumlogit",
        method = "REML")
```

Fixed effects estimation results:

Parametric Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
theta_1	-4.3485	1.5039	-2.8914	0.0039	**
theta_2	0.7500	1.5156	0.4948	0.6208	
standmixed	-0.6175	0.1044	-5.9178	<2e-16	***
fertilizedno	0.5362	0.1901	2.8208	0.0048	**
humus[0cm, 1cm]	-0.1407	0.1648	-0.8536	0.3934	
humus(1cm, 2cm]	0.4421	0.1682	2.6289	0.0086	**
humus(2cm, 3cm]	0.0975	0.1793	0.5439	0.5866	
humus(3cm, 4cm]	0.0771	0.2307	0.3341	0.7383	
moisturemoderately dry	-0.7569	0.2088	-3.6246	0.0003	***
moisturemoderately moist	0.3067	0.1418	2.1625	0.0307	*
alkalivery low	1.1612	0.2482	4.6793	<2e-16	***
alkalilow	-0.3889	0.1881	-2.0680	0.0388	*
alkalihigh	-0.9853	0.2242	-4.3957	<2e-16	***
ph	-0.8074	0.3021	-2.6728	0.0076	**
soil	-0.0470	0.0104	-4.5008	<2e-16	***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Smooth terms:

	Variance	Smooth Par.	df	Stopped
sx(age)	4.9911	0.2004	12.3322	0
sx(canopy)	0.0527	18.9743	4.7092	0
sx(elevation)	0.0668	14.9682	5.0563	0
sx(inclination)	25.8453	0.0387	14.4449	0
sx(year)	0.2971	3.3664	8.4287	0

N = 1793 df = 59.9714 AIC = 1686.69 BIC = 2016.04

logLik = -783.375 GCV = 0.81634 method = REML family = cumlogit

```
R> summary(fm2)
```

Call:

```
bayesx(formula = defoliation ~ stand + fertilized + humus + moisture +
        alkali + ph + soil + sx(age) + sx(inclination) + sx(canopy) +
```



```

sx(year) + sx(elevation) + sx(id, bs = "gs", map = BeechBnd),
data = ForestHealth, family = "cumlogit", method = "REML")

```

Fixed effects estimation results:

Parametric Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
theta_1	-1.8244	2.0034	-0.9106	0.3626
theta_2	4.5302	2.0421	2.2184	0.0267 *
standmixed	-0.1778	0.2269	-0.7835	0.4335
fertilizedno	0.5816	0.4977	1.1685	0.2428
humus[0cm, 1cm]	-0.3371	0.2004	-1.6817	0.0928 .
humus(1cm, 2cm]	0.2453	0.1951	1.2576	0.2087
humus(2cm, 3cm]	0.1656	0.2066	0.8014	0.4230
humus(3cm, 4cm]	0.2205	0.2578	0.8552	0.3926
moisturemoderately dry	-0.7054	0.5450	-1.2943	0.1957
moisturemoderately moist	-0.0765	0.3899	-0.1961	0.8446
alkalivery low	0.9401	0.6297	1.4929	0.1357
alkalilow	-0.3564	0.4866	-0.7324	0.4640
alkalihigh	-0.3869	0.5608	-0.6899	0.4904
ph	-0.3033	0.3611	-0.8399	0.4011
soil	-0.0072	0.0281	-0.2553	0.7985

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Smooth terms:

	Variance	Smooth Par.	df	Stopped
sx(age)	3.8455	0.2600	10.9703	0
sx(canopy)	0.0179	55.8909	3.2481	0
sx(elevation)	0.0002	5203.4900	1.0280	1
sx(id)	56.3986	0.0177	53.6092	0
sx(inclination)	0.0103	97.4621	1.8657	0
sx(year)	0.5220	1.9158	9.1008	0

N = 1793 df = 94.8222 AIC = 1409.33 BIC = 1930.06

logLik = -609.84 GCV = 0.610199 method = REML family = cumlogit

Most of the parametric modeled terms in the second model now have an insignificant effect on tree defoliation, with similar findings for covariates *inclination* and *elevation* (where the pointwise 95% credible intervals cover the zero line). However, the estimate of the *age* effect seems to be improved in terms of monotonicity, see Figure 9.

A kernel density plot of the estimated spatial effect is then obtained by

```
R> plot(fm2, term = "sx(id)", map = FALSE)
```

The effect may also be visualized either using a 3d perspective plot, an image/contour plot or a map effect plot using the boundary file *BeechBnd* with

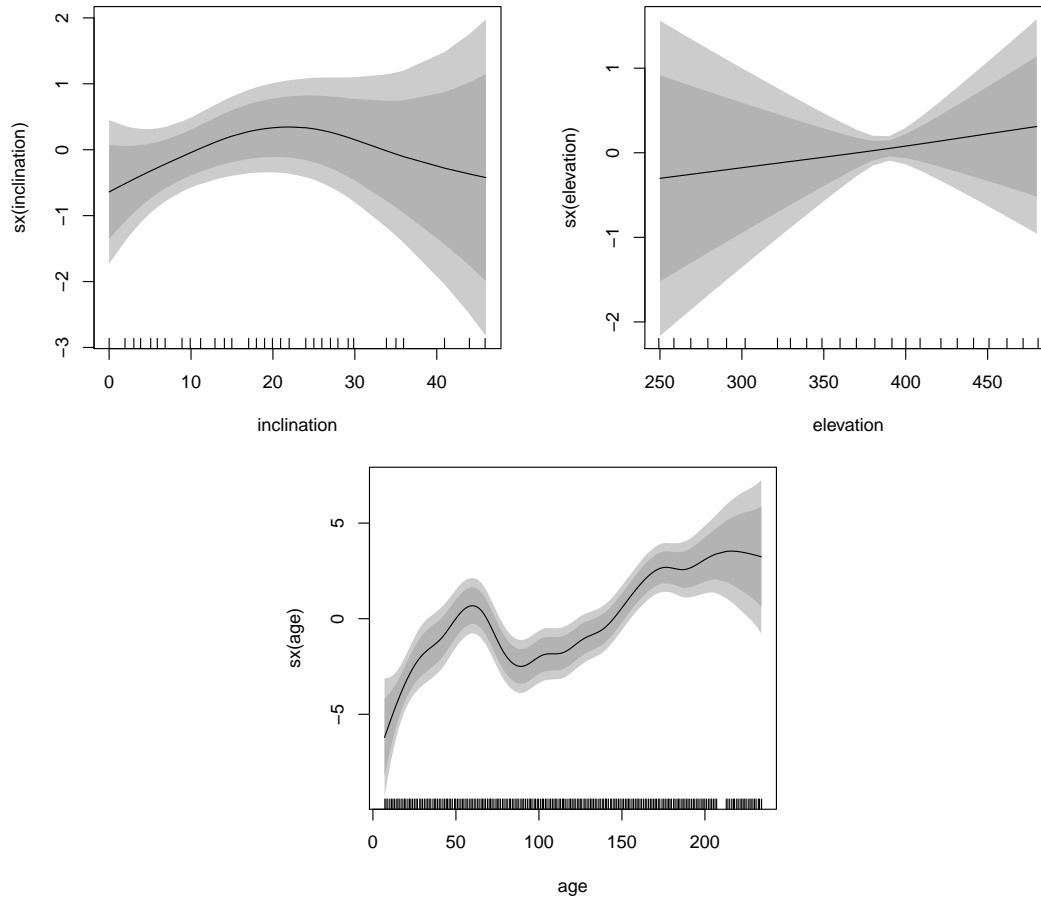


Figure 9: Forest damage: Estimated effects of covariates `inclination`, `elevation` and `age`, including 80% and 95% point-wise confidence intervals, of the model including the spatial effect.

```
R> plot(fm2, term = "sx(id)", map = BeechBnd)
```

Both the kernel density and map effect plot are shown in Figure 10. In this example the coloring of the plot is strongly influenced by a few very high and low values. Therefore, it might be useful to restrict the color range e.g. according to the 10% and 90% quantiles of the kernel density estimate of the effect, by typing

```
R> plot(fm2, term = "sx(id)", map = BeechBnd, range = c(-3, 3))
```

the resulting map is shown in Figure 11. Trimming the color range of the plot now leads to a better representation of the effect.

Summarizing these results identify a strong influence of the spatial effect of the overall model fit, indicating that a clear splitting of locational specific covariates and the spatial effect is hardly possible in this example.

6.3. Childhood malnutrition in Zambia: Analysis with STEP

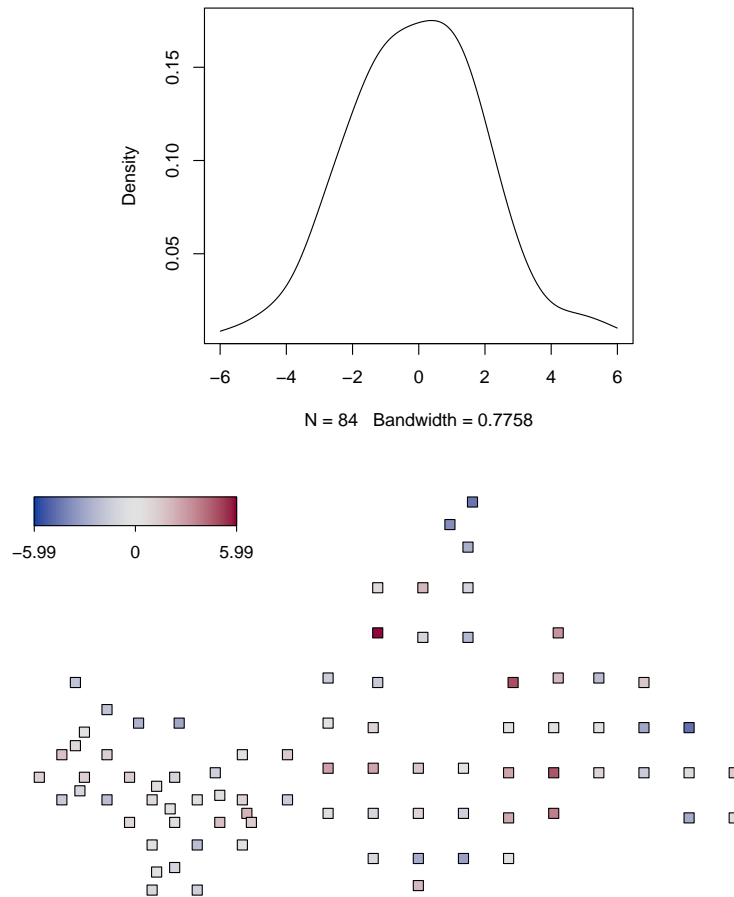


Figure 10: Forest damage: Kernel density estimate of the spatial effect, upper panel, together with a map effect plot, lower panel respectively.

To illustrate the implemented methodology for simultaneous selection of variables and smoothing parameters, we proceed with the dataset on malnutrition in Zambia of Section 6.1. In this example, the structured additive predictor (2) contains two continuous covariates `mbmi` and `agechild`, that are assumed to have a possibly nonlinear effect on the response `stunting` and are modeled with P-splines. However, a linear effect could be more appropriate and, hence, the linear effect is also considered using the selection algorithm in **BayesX**. Additionally, for each variable and function, the implemented procedures decide if a term is included or removed from the model. To estimate the model applying the option `method = "STEP"`, we use the same model formula of Section 6.1 and call

```
R> f <- stunting ~ memployment + urban + gender +
+   sx(education, bs = "factor") + sx(mbmi) + sx(agechild) +
+   sx(district, bs = "mrf", map = ZambiaBnd) + r(district)
R> zms <- bayesx(f, family = "gaussian", method = "STEP",
+   algorithm = "cdescent1", startmodel = "empty",
+   seed = 123, data = ZambiaNutrition)
```

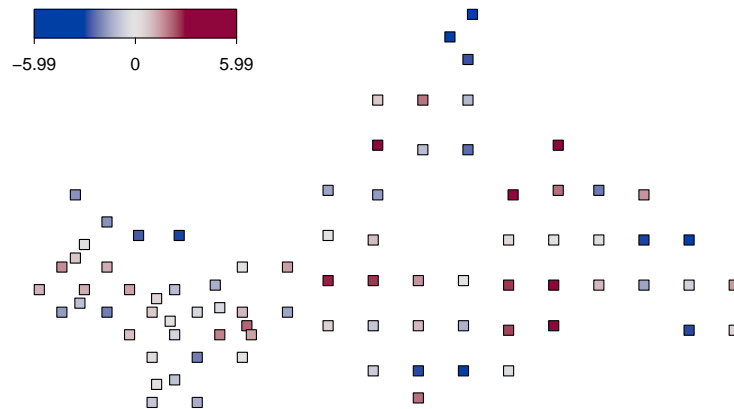


Figure 11: Forest damage: Estimate of the spatial effect with color scaling based on the 10% and 90% quantiles of the kernel density estimate of the effect.

where argument `algorithm` chooses the selection algorithm and `startmodel` the start model for variable selection, see also Table 2 for all possible options. Usually the selected final model is unaffected by the selection algorithm and `startmodel`. However, it is generally of interest to assess the dependence of results on the selection algorithm and the `startmodel`. The summary statistics of the final selected model are then provided with

```
R> summary(zms)
```

Call:

```
bayesx(formula = f, data = ZambiaNutrition, family = "gaussian",
        method = "STEP", algorithm = "cdescent1", startmodel = "empty",
        seed = 123)
```

Fixed effects estimation results:

Parametric Coefficients:

	Mean	Sd	2.5%	50%	97.5%
(Intercept)	-0.5946	0.0000	0.0000	0.0000	0
urbanno	-0.0945	0.0000	0.0000	0.0000	0
genderfemale	0.0589	0.0000	0.0000	0.0000	0
meducation_2	0.1087	0.0000	0.0000	0.0000	0
meducation_3	0.4064	0.0000	0.0000	0.0000	0
mbmi	0.0209	0.0000	0.0000	0.0000	0

Smooth terms:

	lambda	df
f(agechild)	15.4071	10.959
f(district)	7.5775	24.366
r(district)	35.6851	17.872

Scale estimate: 0.7897

N = 4847 AIC_imp = -1024.35 method = STEP family = gaussian

Note that variable `memployment` was removed from the model and variable `mbmi` is modeled by a linear effect. Moreover, the columns `sd`, `2.5%`, `50%` and `97.5%` contain no values, likewise for the estimated random and smooth effects. The posterior quantiles may be computed if argument `CI` in function `bayesx.control()` is specified. E.g. conditional confidence bands can be calculated conditional on the selected model, i.e. they are computed for selected variables and functions only. The computation of conditional confidence bands is based on an MCMC-algorithm subsequent to the selection procedure. For the selection of a model with an subsequent computation of conditional confidence bands the user may type

```
R> zmsccb <- bayesx(f, family = "gaussian", method = "STEP",
+   algorithm = "cdescent1", startmodel = "empty",
+   CI = "MCMCselect", iterations = 10000, step = 10,
+   seed = 123, data = ZambiaNutrition)
```

which results in the following summary

```
R> summary(zmsccb)
```

Call:

```
bayesx(formula = f, data = ZambiaNutrition, family = "gaussian",
  method = "STEP", algorithm = "cdescent1", startmodel = "empty",
  CI = "MCMCselect", iterations = 10000, step = 10, seed = 123)
```

Fixed effects estimation results:

Parametric Coefficients:

	Mean	Sd	2.5%	50%	97.5%
(Intercept)	-0.5906	0.0937	-0.7790	-0.5900	-0.4121
urbanno	-0.0944	0.0242	-0.1398	-0.0947	-0.0457
genderfemale	0.0591	0.0130	0.0337	0.0593	0.0849
meducation_2	0.1087	0.0291	0.0523	0.1083	0.1674
meducation_3	0.4080	0.0690	0.2808	0.4053	0.5448
mbmi	0.0207	0.0041	0.0125	0.0207	0.0289

Smooth terms:

	lambda	df
f(agechild)	15.4071	10.959
f(district)	7.5775	24.366
r(district)	35.6851	17.872

Scale estimate: 0.7897

N = 4847 DIC = 4965.945 pd = 59.33154 AIC_imp = -1024.35
method = STEP family = gaussian iterations = 10000 step = 10

It is also possible to obtain unconditional confidence bands by setting `CI = "MCMCbootstrap"`, which additionally considers the uncertainty due to model selection.

Another important feature of the stepwise procedure is the definition of a `startmodel`, the options are listed in Table 2. Besides the default of an "empty" `startmodel`, it may be reasonable to start with an userdefined model. Therefore, the starting values for the degrees of freedom of the P-spline, spatial and random effect terms need to be specified, by typing

```
R> f <- stunting ~ memployment + urban + gender +
+   sx(education, bs = "factor") + sx(mbmi, dfstart = 2) +
+   sx(district, bs = "mrf", map = ZambiaBnd, dfstart = 5) +
+   r(district, xt = list(dfstart = 5)) +
+   sx(agechild, dfstart = 2)
```

The model is then fitted by

```
R> zmsud <- bayesx(f, family = "gaussian", method = "STEP",
+   algorithm = "cdescent1", startmodel = "userdefined",
+   CI = "MCMCselect", iterations = 10000, step = 10,
+   seed = 123, data = ZambiaNutrition)
```

which actually produces the model output of the first model again.

References

- Belitz C, Brezger A, Kneib T, Lang S (2011). *BayesX – Software for Bayesian Inference in Structured Additive Regression Models. Version 2.0.1*. URL <http://www.stat.uni-muenchen.de/~bayesx>.
- Belitz C, Lang S (2008). “Simultaneous Selection of Variables and Smoothing Parameters in Structured Additive Regression Models.” *Computational Statistics & Data Analysis*, **53**, 61–81.
- Brezger A, Kneib T, Lang S (2005). “**BayesX**: Analyzing Bayesian Structured Additive Regression Models.” *Journal of Statistical Software*, **14**(11), 1–22. URL <http://www.jstatsoft.org/v14/i11/>.
- Brezger A, Lang S (2006). “Generalized Structured Additive Regression Based on Bayesian P-Splines.” *Computational Statistics & Data Analysis*, **50**, 947–991.
- Burnham KP, Anderson DR (1998). *Model Selection and Multimodel Inference*. Springer, New York.
- Chambers JM, Hastie TJ (eds.) (1992). *Statistical Models in S*. Chapman & Hall, London.
- Fahrmeir L, Kneib T, Lang S (2004). “Penalized Structured Additive Regression for Space Time Data: A Bayesian Perspective.” *Statistica Sinica*, **14**, 731–761.
- Fahrmeir L, Kneib T, Lang S (2009). *Regression – Modelle, Methoden und Anwendungen*. 2nd edition. Springer-Verlag, Berlin.

- Fahrmeir L, Tutz G (2001). *Multivariate Statistical Modelling Based on Generalized Linear Models*. Springer-Verlag, New York.
- Fotheringham A, Brunsdon C, Charlton M (2002). *Geographically Weighted Regression: The Analysis of Spatially Varying Relationships*. Wiley, Chichester.
- Göttlein A, Pruscha H (1996). “Der Einfluss von Bestandskenngrößen, Topographie, Standort und Witterung auf die Entwicklung des Kronenzustandes im Bereich des Forstamtes Rothenbuch.” *Forstwissenschaftliches Zentralblatt*, **114**, 146–162.
- Hastie T (2011). **gam**: *Generalized Additive Models*. R package version 1.04.1, URL <http://CRAN.R-project.org/package=gam>.
- Hastie T, Tibshirani R (1990). *Generalized Additive Models*. Chapman & Hall/CRC.
- Hastie T, Tibshirani R (1993). “Varying-Coefficient Models.” *Journal of the Royal Statistical Society B*, **55**, 757–796.
- Hastie TJ, Tibshirani RJ, Friedman J (2009). *The Elements of Statistical Learning*. 2nd edition. Springer, New York.
- Kamman EE, Wand MP (2003). “Geoadditive Models.” *Applied Statistics*, **52**, 1–18.
- Kandala NB, Lang S, Klasen S, Fahrmeir L (2001). “Semiparametric Analysis of the Socio-Demographic and Spatial Determinants of Undernutrition in Two African Countries.” *Research in Official Statistics*, **1**, 81–100.
- Kneib T, Fahrmeir L (2004). “Structured Additive Regression for Multicategorical Space-Time Data: A Mixed Model Approach.” *Biometrics*, **62**, 109–118.
- Kneib T, Heinzl F, Brezger A, Sabanes Bove D (2011). **BayesX**: *R Utilities Accompanying the Software Package BayesX*. R package version 0.2-5, URL <http://CRAN.R-project.org/package=BayesX>.
- Krivobokova T (2009). **AdaptFit**: *Adaptive Semiparametric Regression*. R package version 0.2-2.
- Lin X, Zhang D (1999). “Inference in Generalized Additive Mixed Models by Using Smoothing Splines.” *Journal of the Royal Statistical Society B*, **61**, 381–400.
- Plummer M, Best N, Cowles K, Vines K (2006). “CODA: Convergence Diagnosis and Output Analysis for MCMC.” *R News*, **6**(1), 7–11. URL <http://CRAN.R-project.org/doc/Rnews/>.
- R Development Core Team (2011). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0, URL <http://www.R-project.org/>.
- Rigby RA, Stasinopoulos DM (2005). “Generalized additive models for location, scale and shape,(with discussion).” *Applied Statistics*, **54**, 507–554.
- Ruppert D, Wand MP, Carrol RJ (2003). *Semiparametric Regression*. Cambridge University Press, New York.

- Scheipl F (2011). “**spikeSlabGAM**: Bayesian Variable Selection, Model Choice and Regularization for Generalized Additive Mixed Models in R.” *Journal of Statistical Software*. Under revision.
- Stabler B (2006). *shapefiles: Read and Write ESRI Shapefiles*. R package version 0.6.
- Stasinopoulos DM, Rigby RA (2007). “Generalized Additive Models for Location Scale and Shape (GAMLSS) in R.” *Journal of Statistical Software*, **23**(7), 1–46.
- Wand M (2010). *SemiPar: Semiparametric Regression*. R package version 1.0-3, URL <http://CRAN.R-project.org/package=SemiPar>.
- Wood SN (2006). *Generalized Additive Models: An Introduction with R*. Chapman & Hall/CRC.
- Wood SN (2011a). “Fast stable restricted maximum likelihood and marginal likelihood estimation of semiparametric generalized linear models.” *Journal of the Royal Statistical Society B*, **73**(3), 3–36.
- Wood SN (2011b). *mgcv: GAMs with GCV/AIC/REML Smoothness Estimation and GAMMs by PQL*. R package version 1.7-6, URL <http://CRAN.R-project.org/package=mgcv>.
- Yee TW (2010). “The **VGAM** Package for Categorical Data Analysis.” *Journal of Statistical Software*, **32**(10), 1–34. ISSN 1548-7660. URL <http://www.jstatsoft.org/v32/i10>.
- Yee TW, Wild CJ (1996). “Vector Generalized Additive Models.” *Journal of the Royal Statistical Society B*, **58**(3), 481–493.

A. Appendix

A.1. Installing the BayesX Windows binary

The installation routine `BayesX_windows.exe` (url: http://www.stat.uni-muenchen.de/~bayesx/install/BayesX_windows.exe) may be downloaded from the **BayesX** homepage and executed. The routine will request all necessary information during the installation process. It is recommended to install **BayesX** in a directory without spaces in the path name. This will install a pre-compiled computing kernel including a Java graphical interface, which automatically installs the necessary command-line version of **BayesX** for use within the R interface. The binary is named `bayesx.exe` and is stored in the `commandline` directory of the **BayesX** installation folder.

A.2. Installing the BayesX sources

The zip archive named `bayesxsource.zip` (url: <http://www.stat.uni-muenchen.de/~bayesx/install/bayesxsource.zip>), containing the C++ source code of **BayesX**, needs to be downloaded and unpacked. If the make facility is available, one can simply type `make BayesX` in the shell and **BayesX** will be compiled. Depending on the operating system, some minor modifications of the make file (for example relating to the version of the installed GNU compiler or the location of the readline library) may be necessary. For MAC OS, versions of an adjusted makefile and the main function that have been used for a successful compilation may be found at the FAQ site (<http://www.stat.uni-muenchen.de/~bayesx/bayesxfaq.html>).

A.3. Editing R's profile startup site

To permanently link to the **BayesX** command line binary, R's startup profile site may be edited. See the manual for R's startup mechanism with

```
R> help("Startup")
```

to find out how to edit the startup site on specific systems that is processed at the beginning of a new R session. Then, by adding the line

```
options(bayesx.bin = "path/to/BayesX")
```

to the startup site will tell R where to find the binary permanently. The string `"path/to/BayesX"` is the full path to the **BayesX** binary with the name of the binary at last. On Windows systems the binary name is `"bayesx.exe"`, on all other systems usually `"BayesX"`. Hence, for Windows platforms `bayesx.bin` may be specified e.g. with

```
options(bayesx.bin = "C:/BayesX/commandline/bayesx.exe")
```

depending on the installation location of the binary.

Furthermore, another possibility is to add the installation directory of the binary to the environment `PATH` variable of the operating system. Both options will automatically link the binary with R for the upcoming sessions.

A.4. Most important arguments used within function `plot.bayesx()`

Argument	Description
<code>term</code>	the term that should be plotted, either an integer or a character, e.g. <code>term = "sx(x)"</code> .
<code>which</code>	choose the type of plot that should be drawn, possible options are: <code>"effect"</code> , <code>"coef-samples"</code> , <code>"var-samples"</code> , <code>"intcpt-samples"</code> , <code>"hist-resid"</code> , <code>"qq-resid"</code> , <code>"scatter-resid"</code> , <code>"scale-resid"</code> , <code>"max-acf"</code> . Argument <code>which</code> may also be specified as integer, e.g. <code>which = 1</code> . The first three arguments are all model term specific. For the residual model diagnostic plot options <code>which</code> may be set with <code>which = 5:8</code> .
<code>residuals</code>	if set to <code>TRUE</code> , partial residuals may also be plotted if available.
<code>rug</code>	if set to <code>TRUE</code> , a <code>rug()</code> is added to the plot.
<code>jitter</code>	if set to <code>TRUE</code> , a <code>jitter()</code> ed <code>rug()</code> is added to the plot.
<code>col.surface</code>	the color of the surface, may also be a function, e.g. <code>col.surface = heat.colors</code> .
<code>grid</code>	the grid size of the surface(s).
<code>image</code>	if set to <code>TRUE</code> , an <code>image.plot()</code> is drawn.
<code>contour</code>	if set to <code>TRUE</code> , a <code>contour()</code> plot is drawn.
<code>map</code>	the map to be plotted, the map object must be a list of matrices with first column indicating the x -coordinate and second column the y -coordinate each, see also function <code>polygon()</code> .
<code>legend</code>	if set to <code>TRUE</code> , a legend will be shown.
<code>range</code>	specify the range of values the plot should be generated for, e.g. only values between -2 and 2 are of interest then <code>range = c(-2, 2)</code> .
<code>color</code>	the colors for the legend, may also be a function, e.g. <code>colors = heat.colors</code> .
<code>pos</code>	the position of the legend, either a numeric vector, e.g. <code>pos = c(0.1, 0.2)</code> will add the legend at the 10% point in the x -direction and at the 20% point in the y -direction of the plotting window, may also be negative, or one of the following: <code>"bottomleft"</code> , <code>"topleft"</code> , <code>"topright"</code> or <code>"bottomright"</code> . Using function <code>plotmap()</code> option <code>"right"</code> is also valid.
<code>lrange</code>	specifies the range of the legend.
<code>symmetric</code>	if set to <code>TRUE</code> , a symmetric legend will be drawn corresponding to the $+ - \max(x)$ of values x that are used for plotting.

Table 7: Most important plotting parameters using the generic function `plot.bayesx()`. The first block describes arguments of `plot.bayesx()`, subsequent blocks arguments that are passed to function `plot2d()`, `plot3d()`, `plotmap()` and `colorlegend()` respectively.

Affiliation:

Nikolaus Umlauf, Stefan Lang, Achim Zeileis

Department of Statistics

Universität Innsbruck

Universitätsstr. 15

A-6020 Innsbruck, Austria

E-mail: Nikolaus.Umlauf@uibk.ac.at,

Stefan.Lang@uibk.ac.at,

Achim.Zeileis@R-project.org

URL: <http://www.uibk.ac.at/statistics/personal/umlauf/>,

<http://www.uibk.ac.at/statistics/personal/lang/>,

<http://eeecon.uibk.ac.at/~zeileis/>

Thomas Kneib

Department of Mathematics

Universität Oldenburg

D-26111 Oldenburg, Germany

E-mail: Thomas.Kneib@uni-oldenburg.de

URL: <http://www.staff.uni-oldenburg.de/thomas.kneib/>