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Structured Additive Regression Models: An R Interface to BayesX

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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 remainder 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

```
\mathtt{stunting}_i = \gamma_0 + f_1(\mathtt{agechild}_i) + f_2(\mathtt{mbmi}_i) + f_{spat}(\mathtt{district}_i) + \varepsilon_i, \qquad \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

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

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) 0.0274 0.0400 -0.0551 0.0271 0.1049
```

Smooth terms variances:

```
Mean Sd 2.5% 50% 97.5% Min Max sx(agechild) 0.0068 0.0070 0.0013 0.0049 0.0229 0.0006 0.0892 sx(district) 0.0453 0.0182 0.0207 0.0410 0.0885 0.0127 0.1502 sx(mbmi) 0.0022 0.0034 0.0003 0.0012 0.0094 0.0002 0.0483
```

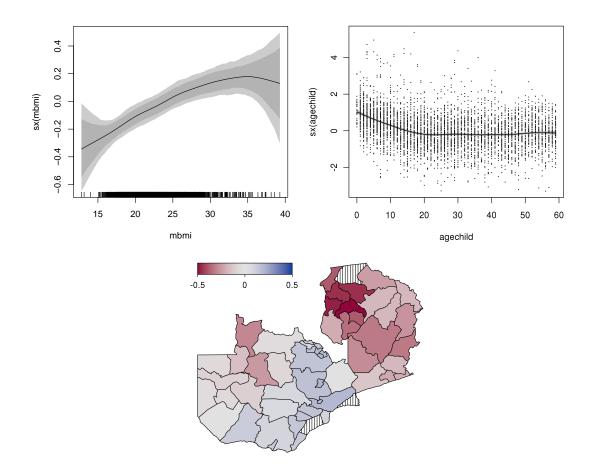


Figure 1: Visualization examples: Estimated effect for covariate mbmi (black line) together with 95% and 80% credible intervals (upper left panel). The upper right panel shows the estimated effect of agechild including partial residuals. The lower panel illustrates visualization of the estimated spatial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

Scale estimate:

Mean Sd 2.5% 50% 97.5% Sigma2 0.8174 0.0168 0.7847 0.8171 0.8514

N = 4847 burnin = 2000 DIC = 4887.417 pd = 38.27104 method = MCMC family = gaussian iterations = 12000 step = 10

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

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

where h is a known link function and γ 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

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

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, \ldots, 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: $f_i(\mathbf{z}) = z_1 f_{spat}(z_s)$ or $f_i(\mathbf{z}) = z_1 f(z_2, z_3)$,
- random intercepts with cluster index c: $f_i(\mathbf{z}) = \beta_c$,
- random slopes with cluster index c: $f_i(\mathbf{z}) = z_1 \beta_c$.

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

$$\mathbf{f}_i = \mathbf{Z}_i \boldsymbol{\beta}_i$$

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

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

where **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_i is

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

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 $\boldsymbol{\beta}_j$ 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 an 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 Carrol 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 \$3 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 \mathbf{BayesX} . Next to the integration of function $\mathbf{s}()$, a more \mathbf{BayesX} alike model term constructor function is provided. The advantage is that a common \mathbf{BayesX} user may specify models in a more familiar way, which will make a change to $\mathbf{R2BayesX}$ more easy. The function is called $\mathbf{sx}()$ and is described in Section 5.4. To avoid package conflicts the new function simply interfaces function $\mathbf{s}()$. 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 <code>install.bayesx()</code>. 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 $\mathbf{R2BayesX}$ is called $\mathtt{bayesx}()$. The arguments of $\mathtt{bayesx}()$ 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 \$3 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-	"MCMC" "REML" "STEP"
		link	
"cox"	continuous-time sur-		"MCMC" "REML"
	vival data		
"cumprobit"	cumulative threshold	probit	"MCMC" "REML"
"multistate"	continuous-time multi-		"MCMC" "REML"
	state data		
"binomialcomploglog"	binomial	compl.	"REML"
		log-log	
"cumlogit"	cumulative multinomial	logit	"REML"
"multinomialcatsp"	unordered multinomial	logit	"REML"
	(with category-specific		
	covariates)		
"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				
	iterations	integer, sets the number of iterations for the sampler, default:				
		12000.				
un an au	burnin	integer, sets the burn-in period of the sampler, default: 2000.				
"MCMC"	step	integer, defines the thinning parameter for MCMC simulation.				
		E.g., step = 50 means, that only every 50th sampled param-				
		eter will be stored and used to compute characteristics of t				
		posterior distribution as means, standard deviations or quan-				
		tiles, default: 10.				
	eps	numeric, defines the termination criterion of the estimation				
		process. If both the relative changes in the regression coef-				
		ficients and the variance parameters are less than eps, the				
II DEMI II	estimation process is assumed to have converged					
"KEML"		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				

continue	ed from previou	ıs page
	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 gam function of S-plus, see Chambers and Hastie 1992), default: "cdescent1".
"STEP"	criterion	character, specifies the goodness of fit criterion, possible criterions 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 euqal 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
print()	simple printed display of the initial call and some additional in-
	formation of the fitted model.
summary()	returns an object of class "summary.bayesx" containing the rele-
	vant summary statistics (which has a print() method).
coef()	extracts coefficients of the linear modeled terms.
<pre>confint()</pre>	compute confidence intervals of linear modeled terms if method =
	"REML", for "MCMC" the quantiles of the coefficient samples accord-
	ing to a specified probability level are computed.
cprob()	extract contour probabilities of a particular P-spline term, only
	meaningful if method = "MCMC" and argument contourprob is
	specified as an additional argument in the term constructor func-
	tion sx(), or within argument xt in function s(). E.g. in
	the introductory example, contour probabilities for the term us-
	ing covariate mbmi are estimated with s(mbmi, bs = "ps", xt =
	list(contourprob = 4)) (see also Section 5.4).
fitted()	fitted values of either the mean and linear predictor, or a selected
	model term.
<pre>bayesx_logfile(),</pre>	extracts the internal BayesX log file, the program file and the
<pre>bayesx_prgfile(),</pre>	overall runtime of the binary.
<pre>bayesx_runtime()</pre>	
residuals()	extract model or partial residuals for a selected term.
samples()	extract samples of parameters from MCMC simulation.
terms()	extract terms of model components.
model.frame()	extract/generate a model frame.
logLik()	extract fitted log-likelihood, only if method = "REML".
plot()	either model diagnostic plots or effect plots of particular terms.
<pre>getscript()</pre>	generate an R script for term effect, diagnostic plots and model
	summary statistics.
AIC(), BIC(),	computes information criteria, availability is dependent on the
DIC(), GCV()	method 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 <code>getscript()</code>. 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 <code>R2BayesX</code> 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 $\eta = \ldots + g_1(z_1)z + g_2(z_2)z + \gamma_0 + \gamma_1 z + \ldots$ are not identified, whereas in $\eta = \ldots + g_1(z_1)z + \gamma_0 + \ldots$, 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",	P-spline with first or second order difference penalty.
"psplinerw1",	
"psplinerw2"	
"te",	defines a two-dimensional P-spline based on the tensor product
"pspline2dimrw1"	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 with stationary Gaussian random fields: estimates
"geokriging"	a stationary Gaussian random field based on the centroids of a map object provided in boundary format (see function read.bnd() and shp2bnd()) as an additional argument named map within function sx(), or supplied within argument xt when using function s(), e.g. xt = list(map = MapBnd).
"gs",	geosplines based on two-dimensional P-splines with first order
"geospline"	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. Estima- tion is based on the coordinates of the centroids of the regions of a map object provided in boundary format (see function read.bnd() and shp2bnd()) as an additional argument named map within function sx(), or supplied within argument xt when using function s(), e.g. xt = list(map = MapBnd).
"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 read.bnd(), read.gra() and shp2bnd()), as an additional ar-
	gument named map within function sx(), or supplied within argument xt when using function s(), e.g. xt = list(map = MapBndorGra).
	continued on next page

continued from prev	ious 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 $\log(\lambda(time))$.
"factor"	special BayesX specifier for factors, especially meaningful if
	method = "STEP", since the factor term is then treated as a
	full term, which is either included or removed from the model.
"ridge", "lasso",	shrinkage of fixed effects: defines a shrinkage-prior for the cor-
"nigmix"	responding parameters γ_j , $j = 1,, q, q \ge 1$ of the linear
	effects x_1, \ldots, 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 <code>bayesx()</code> may be sufficient. However, the interfacing functions that are consecutively called within <code>bayesx()</code> can also be used independently. This could be meaningful for two reasons: First, users may want to use already existing <code>BayesX</code> program files wherefore a new setup within R is not required, and secondly, there might be a need for automated importing of <code>BayesX</code> 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))</pre>
```

```
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

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

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

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

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

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

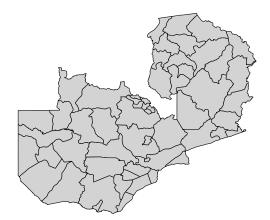


Figure 2: Example on childhood malnutrition: A simple map of the districts in Zambia.

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)</pre>
```

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)</pre>
```

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)
```

Fixed effects estimation results:

Parametric Coefficients:

	Mean	Sd	2.5%	50%	97.5%
(Intercept)	0.0991	0.0475	0.0046	0.1018	0.1863
memploymentno	-0.0084	0.0135	-0.0359	-0.0084	0.0170
urbanno	-0.0895	0.0217	-0.1306	-0.0893	-0.0450
genderfemale	0.0582	0.0133	0.0320	0.0578	0.0850
meducationno	-0.1722	0.0269	-0.2248	-0.1719	-0.1163
meducationprimary	-0.0611	0.0262	-0.1115	-0.0614	-0.0091

Smooth terms variances:

```
Mean Sd 2.5% 50% 97.5% Min Max sx(agechild) 0.0062 0.0060 0.0014 0.0042 0.0233 0.0007 0.0570 sx(district) 0.0360 0.0191 0.0094 0.0325 0.0813 0.0025 0.1784 sx(mbmi) 0.0019 0.0028 0.0003 0.0011 0.0081 0.0002 0.0468
```

Random effects variances:

```
Mean Sd 2.5% 50% 97.5% Min Max r(district) 0.0076 0.0064 0.0008 0.0062 0.0226 0.0003 0.0701
```

Scale estimate:

```
Mean Sd 2.5% 50% 97.5% Sigma2 0.8023 0.0163 0.7721 0.8017 0.836
```

```
N = 4847 burnin = 2000 DIC = 4899.506 pd = 50.41262 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 <code>agechild</code> and <code>mbmi</code> 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

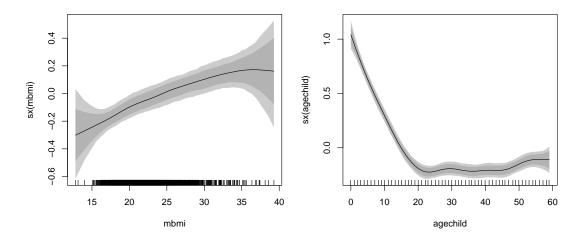


Figure 3: Example on childhood malnutrition: Effect of the body mass index of the child's mother and of the age of the child together with pointwise 80% and 95% credible intervals.

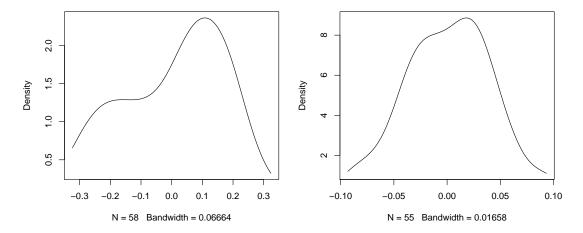


Figure 4: Example on childhood malnutrition: Kernel density estimates of the mean of the structured, left panel, and the unstructured spatial effect, right panel respectively.

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

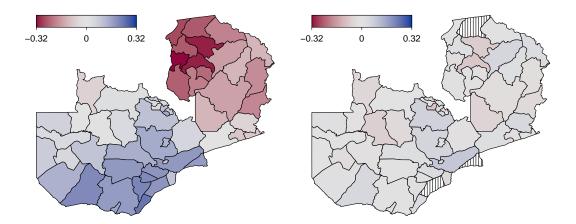


Figure 5: Example on childhood malnutrition: Estimated mean effect of the structured spatial effect (left panel), together with the unstructured spatial effect using the color and legend scaling of the structured effect (right panel).

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 unstructered 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 unstructered 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")
```

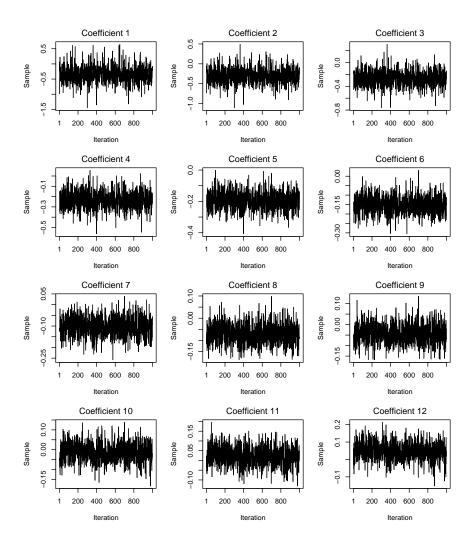


Figure 6: Example on childhood malnutrition: Sampling paths of the first 12 coefficients of term sx(mbmi).

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 ore even 32000 iterations).

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

R> bayesx_logfile(zm)

> bayesreg b

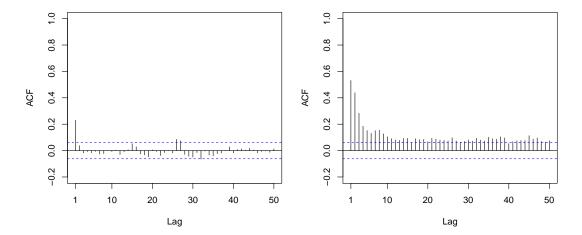


Figure 7: Example on childhood malnutrition: Autocorrelation function of the samples of the variance parameter of term sx(mbmi), left panel, maximum autocorrelation of all parameters of the model, right panel respectively.

```
> 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 + meducationno +
 meducationprimary, 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, 'de-
	foliation $< 12.5\%$ ', ' $12.5\% \le defoliation < 50\%$ ' and 'defoli-
	ation $\geq 50\%$ '.
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', 'moder-
	ately 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

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

where f_1, \ldots, f_5 are possibly nonlinear smooth functions of the continuous covariates and $\mathbf{x}'_{it}\gamma$ 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)</pre>
```

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)</pre>
```

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

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)</pre>
```

Taking a look at model information criteria with

```
R> BIC(fm1, fm2)

df BIC
fm1 59.9714 2016.04
fm2 94.8222 1930.06
```

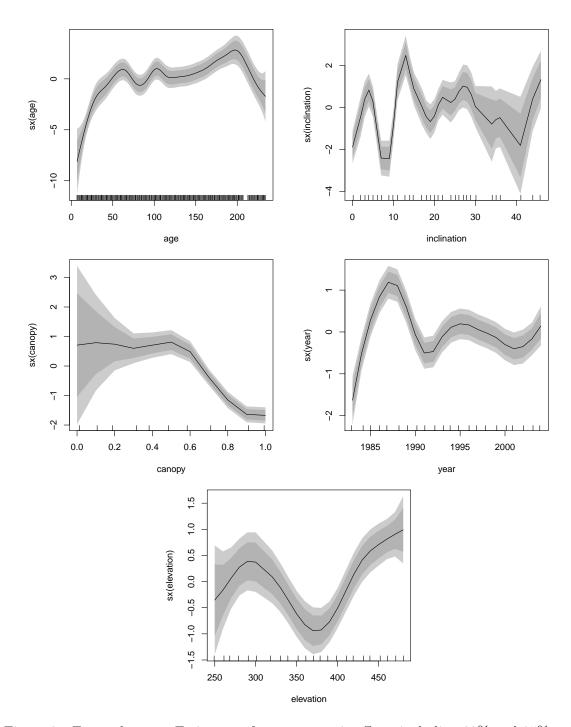


Figure 8: Forest damage: Estimates of nonparametric effects including 80% and 95% pointwise confidence intervals of the model without the spatial effect.

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
<pre>sx(elevation)</pre>	0.0668	14.9682	5.0563	0
<pre>sx(inclination)</pre>	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:

	${\tt Estimate}$	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
<pre>sx(elevation)</pre>	0.0002	5203.4900	1.0280	1
sx(id)	56.3986	0.0177	53.6092	0
<pre>sx(inclination)</pre>	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

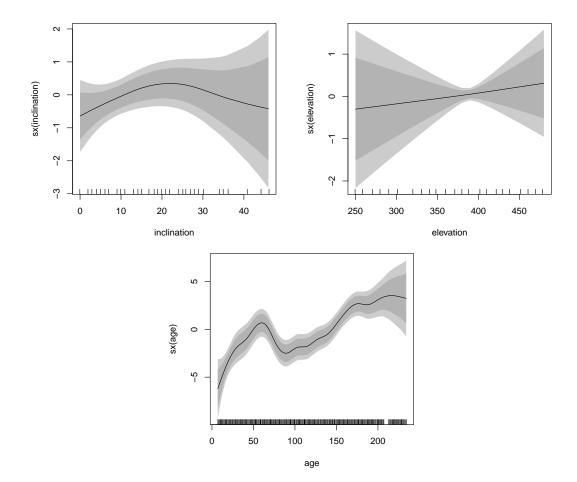


Figure 9: Forest damage: Estimated effects of covariates inclination, elevation and age, including 80% and 95% point-wise confidence intervals, of the model including the spatial effect.

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

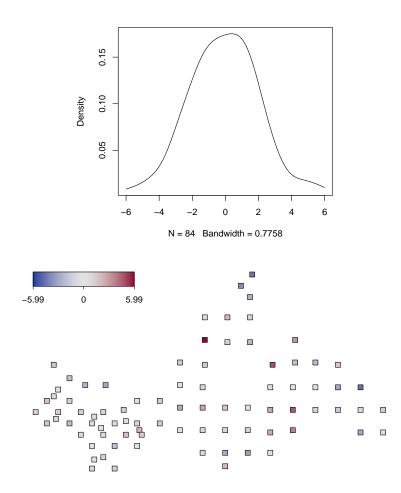


Figure 10: Forest damage: Kernel density estimate of the spatial effect, upper panel, together with a map effect plot, lower panel respectively.

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(meducation, 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)</pre>
```

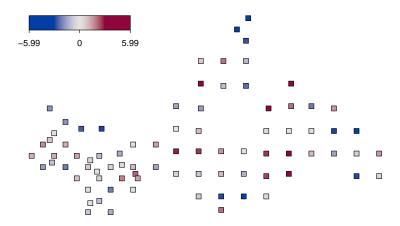


Figure 11: Forest damage: Estimate of the spatial effect with color scaling based on the 10% and 90% quantiles of the kernel density estimate of the effect.

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
${\tt genderfemale}$	0.0589	0.0000	0.0000	0.0000	0
${\tt meducation_2}$	0.1087	0.0000	0.0000	0.0000	0
${\tt meducation_3}$	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

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
            -0.0944 0.0242 -0.1398 -0.0947 -0.0457
urbanno
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

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

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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
term	the term that should be plotted, either an integer or a char-
	acter, e.g. term = "sx(x)".
which	choose the type of plot that should be drawn, possible
	options are: "effect", "coef-samples", "var-samples",
	"intcpt-samples", "hist-resid", "qq-resid",
	"scatter-resid", "scale-resid", "max-acf". Argu-
	ment which may also be specified as integer, e.g. which =
	1. The first three arguments are all model term specific.
	For the residual model diagnostic plot options which may
	be set with which = 5:8.
residuals	if set to TRUE, partial residuals may also be plotted if avail-
	able.
rug	if set to TRUE, a rug() is added to the plot.
jitter	if set to TRUE, a jitter()ed rug() is added to the plot.
col.surface	the color of the surface, may also be a function, e.g.
	col.surface = heat.colors.
grid	the grid size of the surface(s).
image	if set to TRUE, an image.plot() is drawn.
contour	if set to TRUE, a contour() plot is drawn.
map	the map to be plotted, the map object must be a list of matri-
	ces with first column indicating the x-coordinate and second
3 3	column the y-coordinate each, see also function polygon().
legend	if set to TRUE, a legend will be shown.
range	specify the range of values the plot should be generated for,
	e.g. only values between -2 and 2 are of interest then range
color	= c(-2, 2). the colors for the legend, may also be a function, e.g. colors
COTOL	= heat.colors.
pos	the position of the legend, either a numeric vector, e.g. pos =
pos	c(0.1, 0.2) will add the legend at the 10% point in the x -
	direction and at the 20% point in the y -direction of the plot-
	ting window, may also be negative, or one of the following:
	"bottomleft", "topleft", "topright" or "bottomright".
	Using function plotmap() option "right" is also valid.
lrange	specifies the range of the legend.
symmetric	if set to TRUE, a symmetric legend will be drawn correspond-
	ing 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.

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