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# Structured Additive Regression Models: An R Interface to BayesX

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# Overview

- Introduction
- Structured Additive Regression Models (STAR)
- Installing the **BayesX** binary
- The main model fitting function
- More components of the interface
- Available additive terms
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- References

# Introduction: What is BayesX?

The free software **BayesX** is a standalone program comprising powerful tools for Bayesian and mixed model based inference in complex semiparametric regression models with structured additive predictor (STAR).

- Generalized additive models (GAM).
- Generalized additive mixed models (GAMM).
- Generalized geoadditive mixed models (GGAMM).
- Dynamic models.
- Varying coefficient models (VCM).
- Geographically weighted regression.

**BayesX** is written in C++ and utilizes numerically efficient (sparse) matrix architectures.

# Introduction: What is BayesX?

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

1. Full Bayesian inference via MCMC.
2. Inference via a mixed model representation.
3. Penalized likelihood including variable selection.

**BayesX** provides functionality for the following types of responses:

- Univariate exponential family.
- Categorical responses with unordered responses.
- Categorical responses with ordered responses.
- Continuous time survival models.
- Continuous time multi-state models.

# Introduction: The R interface

**Problems: BayesX** only provides limited functionality for

- handling/manipulating data sets,
- handling/manipulating geographical maps,
- exploring/visualizing estimation results.

Therefore, the R package **BayesX** (available at CRAN) was developed, which provides functionality for exploring and visualizing estimation results.

However, estimating models from **BayesX** with special program files and handling estimation outputs within R is still time consuming and not straightforward.

# Introduction: The R interface

**Now:** New interface package **R2BayesX** for

- specifying/estimating STAR models with **BayesX** directly from R,
- standard methods and extractor functions for **BayesX** fitted model objects, e.g. producing high level graphics of estimated effects, model diagnostic plots, summary statistics and more.

In addition:

- Run already existing **BayesX** input program files from R.
- Automatically import **BayesX** output files into R.

To install the package directly within R type:

```
install.packages("R2BayesX",
  repos = "http://R-Forge.R-project.org")
```

# Introduction: Example

**Dataset on malnutrition in Zambia:**
The main interest is to model the dependence of `stunting` of newborn children on covariates including

- the age of the child in months (`agechild`),
- the mother's bmi (`mbmi`)
- and the `district` the mother lives in.

We start with the following model:

$$\texttt{stunting}_i = \gamma_0 + f_1(\texttt{agechild}_i) + f_2(\texttt{mbmi}_i) + f_{spat}(\texttt{district}_i) + \varepsilon_i,$$

with $\varepsilon_i \sim N(0, \sigma^2)$.

# Introduction: Example

Loading the data and boundary object

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

The model is specified using R's formula language definition

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

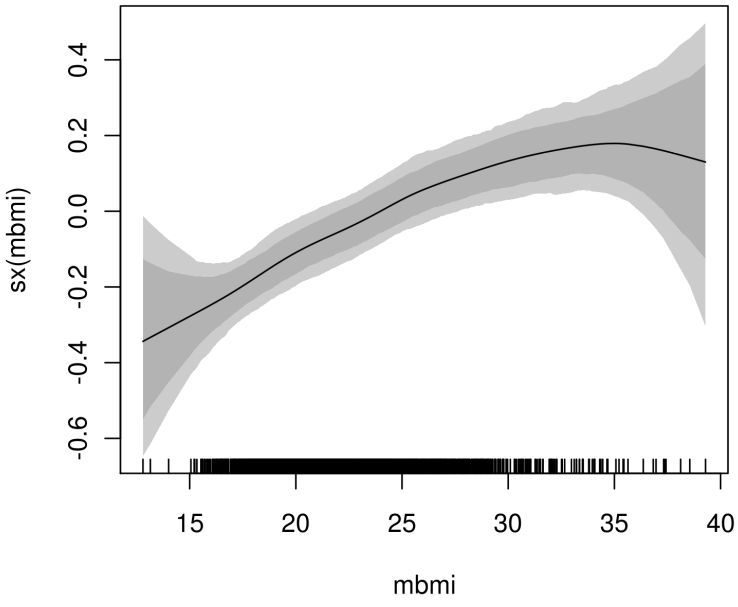
estimated by

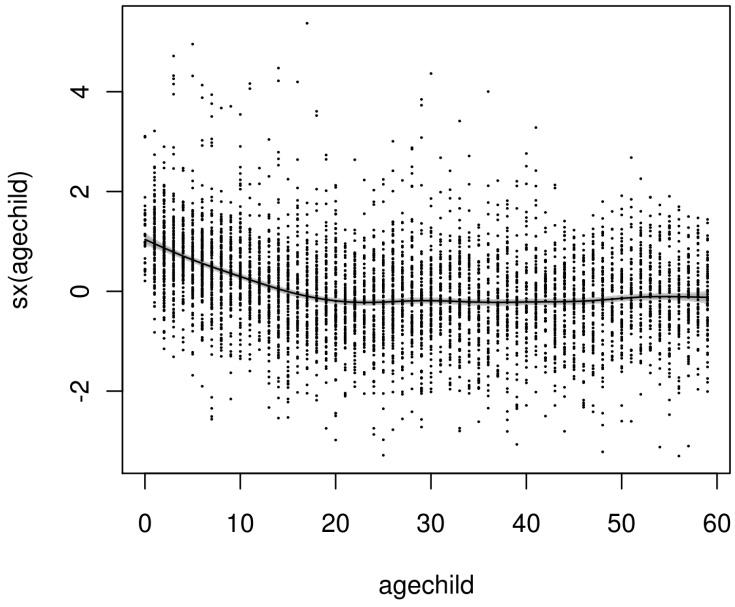
```
R> b <- bayesx(f, family = "gaussian", method = "MCMC",
+     data = ZambiaNutrition)
```

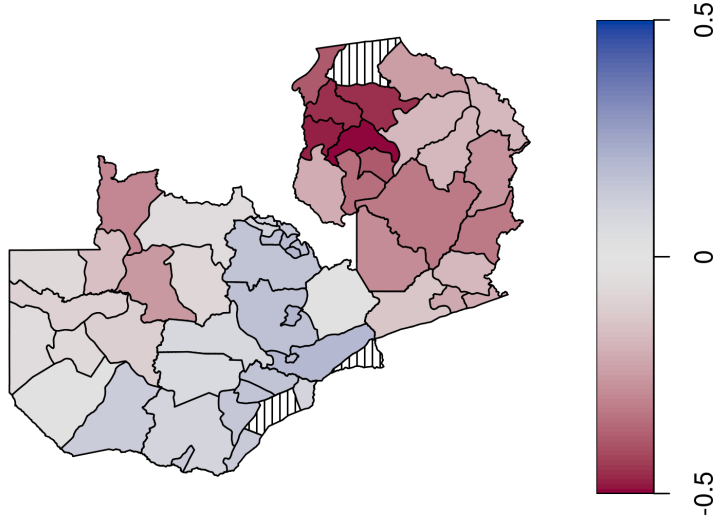
and plotted, e.g. by typing

```
R> plot(b, map = ZambiaBnd)
```

# Introduction: Example



# STAR models

Distributional and structural assumptions, given covariates and parameters, are based on generalized linear models with

$$E(y|\mathbf{x}, \mathbf{z}, \gamma, \boldsymbol{\theta}) = h^{-1}(\eta)$$

and structured additive predictor

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

- $\mathbf{x}'\gamma$ parametric part of the predictor.
- $\mathbf{z}$ represents a generic vector of all nonlinear modeled covariates, e.g. may include continuous covariates, time scales, location or unit or cluster indexes.
- The vector $\boldsymbol{\theta}$ comprises all parameters of the functions $f_1, \ldots, f_p$.
- $f_j$ one-/two-/higher-dimensional, not necessarily continuous functions.

# STAR models: Modeling the functions $f_j$

The functions $f_j$ are possibly smooth functions comprising effects (and combinations) as e.g. given by:

- Nonlinear effects of continuous covariates.
- Two-dimensional surfaces.
- Spatially correlated effects.
- Varying coefficients.
- Spatially varying effects.
- Random intercepts.
- Random slopes.

# STAR models: General form

- Vector of function evaluations $\mathbf{f}_j = (f_j(\mathbf{z}_1), \ldots, f_j(\mathbf{z}_n))$ of the $i = 1, \ldots, n$ observations can be written in matrix notation

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

  with $\mathbf{Z}_j$ as the design matrix, where $\boldsymbol{\beta}_j$ are unknown regression coefficients.
- Form of $\mathbf{Z}_j$ only depends on the functional type chosen.
- Penalized least squares:

$$\text{PLS}(\boldsymbol{\beta}, \boldsymbol{\gamma}) = ||\mathbf{y} - \boldsymbol{\eta}||^2 + \lambda_1 \boldsymbol{\beta}_1' \mathbf{K}_1 \boldsymbol{\beta}_1 + \ldots + \lambda_p \boldsymbol{\beta}_p' \mathbf{K}_p \boldsymbol{\beta}_p$$

# STAR models: General form

- Prior for $\beta$ in the corresponding Bayesian approach

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

  $\tau_j^2$ variance parameter, governs the smoothness of $f_j$.
- Structure of $\mathbf{K}_j$ also depends on the type of covariates and on assumptions about smoothness of $\mathbf{f}_j$.
- The variance parameter $\tau_j^2$ is equivalent to the inverse smoothing parameter in a frequentist approach. Utilizing mixed model technology, restricted maximum likelihood (REML) forms a basis for determination. From a Bayesian perspective, this yields empirical Bayes/posterior mode estimates for the STAR models.

# Installing the BayesX binary

For model fitting with package **R2BayesX**, the binary command-line version of **BayesX** needs to be installed and linked to R first.

```
R> library("R2BayesX")
R> install.bayesx(inst.dir = "/path/to/bin", source.dir = NULL)
```

Then by setting e.g.

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

the model fitting function of **R2BayesX** will know the location of the binary using function `getOption()`.

**Note:** on Windows, function `install.bayesx()` will download and execute an installer, which also installs the GUI version of **BayesX**.

# The main model fitting function

The arguments of the main model fitting function are

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

**Families:**

`"binomial"`, `"binomialprobit"`, `"gamma"`, `"gaussian"`,
`"multinomial"`, `"poisson"`, `"cox"`, `"cumprobit"`, `"multistate"`,
`"binomialcomploglog"`, `"cumlogit"`, `"multinomialcatsp"`,
`"multinomialprobit"`, `"seqlogit"`, `"seqprobit"`.

**Methods:**

`"MCMC"`, `"REML"`, `"STEP"`.

**Note:** `family` objects are currently not supported.

# More components of the interface

Internally, function `bayesx()` calls the following functions:

1. `parse.bayesx.input()`
2. `write.bayesx.input()`
3. `run.bayesx()`
4. `read.bayesx.output()`

These functions are operating independently and may also be called by the R user.

The functionality is especially helpful for already existing **BayesX** program and output files.

Moreover, function `read.bayesx.output()` also returns objects of class `"bayesx"`.

# Available additive terms

The main model term constructor function is function `sx()`, with arguments:

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

`sx()` is simply an interface to function `s()` from package **mgcv**.

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

Random effects are included in the models using function `r()`.

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

**Basis/term types:**

`"rw1"`, `"rw2"`, `"season"`, `"ps"` (`"psplinerw1"`, `"psplinerw2"`), `"te"` (`"pspline2dimrw1"`), `"kr"` (`"kriging"`), `"gk"` (`"geokriging"`), `"gs"` (`"geospline"`), `"mrf"` (`"spatial"`), `"bl"` (`"baseline"`), `"factor"`, `"ridge"`, `"lasso"`, `"nigmix"`.

# Available additive terms

Additional options within "`...`" and `xt` for each basis/term type and method may be looked up using function `bayes.term.options()`, e.g.

```
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'.

      order: only if 'bs = "ps"', the order of the
           difference penalty.
           Default: integer, 'order = 2'.
        .
        .
        .
```

# Illustration

Following Kandala, Lang, Klasen and Fahrmeir (2001), the task is to model `stunting` of newborn children on the following covariates:

| 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` | Is the mother employed? |
| `meducation` | Mother's educational status. |
| `urban` | Is the domicile in an urban region? |
| `gender` | Gender of the child. |

The predictor of the STAR model is given by

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

# Illustration

The formula is set 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> set.seed(321)
R> zm <- bayesx(f, family = "gaussian", method = "MCMC",
+     data = ZambiaNutrition, iterations = 12000, burnin = 2000,
+     step = 10)
```

Model summary

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

# Illustration

```
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
```

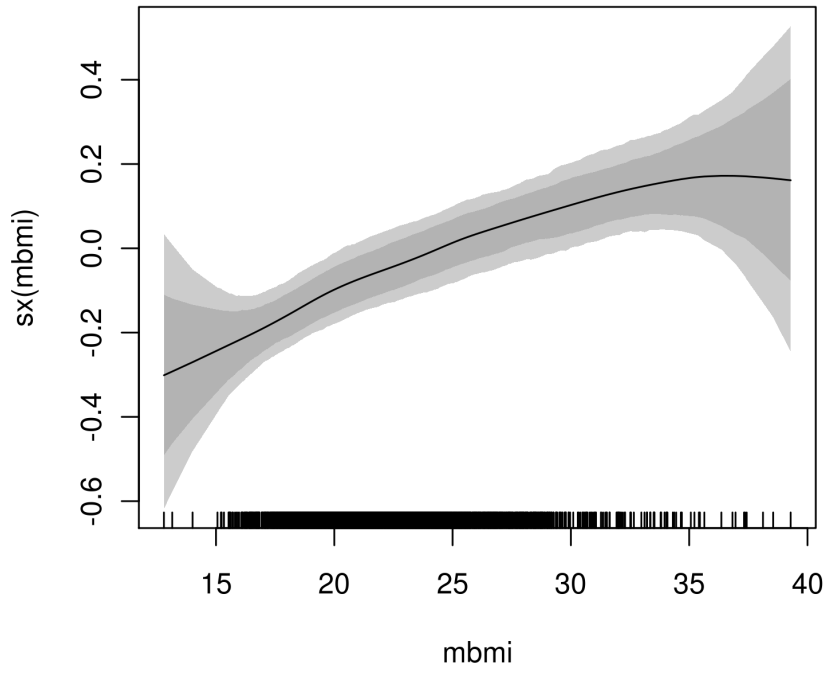
# Illustration

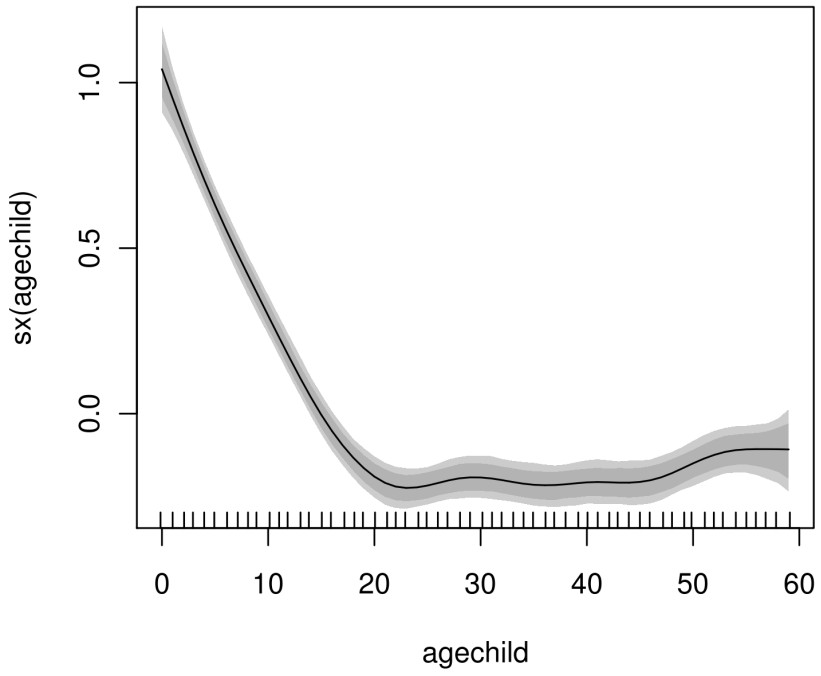
```
Random effects variances:
               Mean     Sd   2.5%    50%  97.5%    Min    Max
r(district) 0.0076 0.0064 0.0008 0.0062 0.0226 0.0003 0.0701

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
```

# Illustration

Plotting of specific terms

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

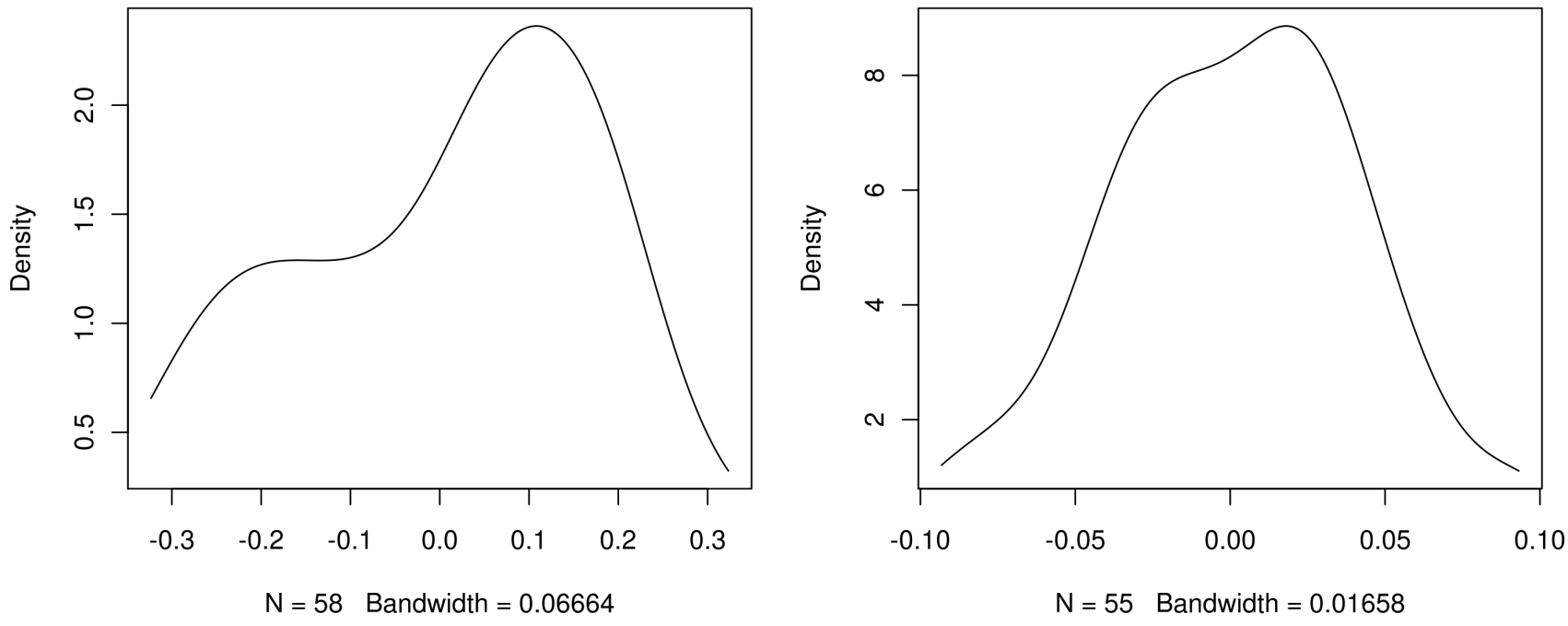


# Illustration

Spatial effects, kernel density estimates

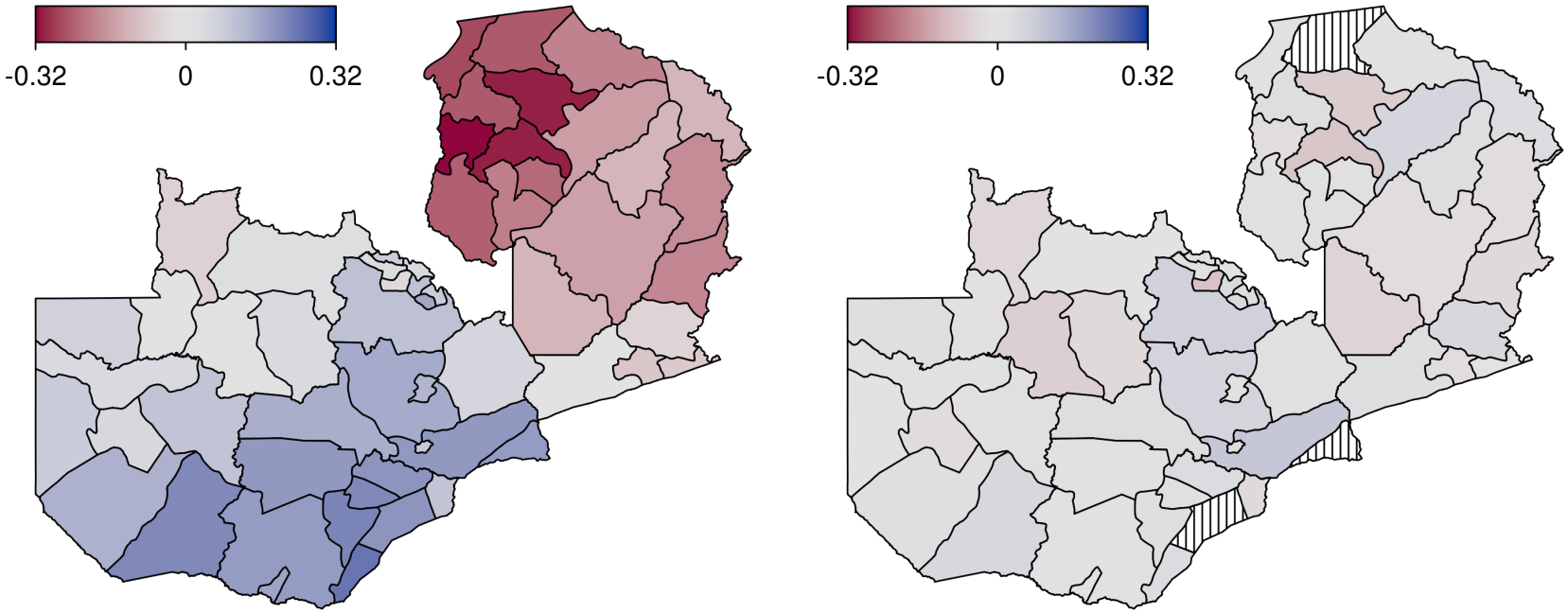
```
R> plot(zm, term = c("sx(district)", "r(district)"))
```



# Illustration

Spatial effects, map effect plots

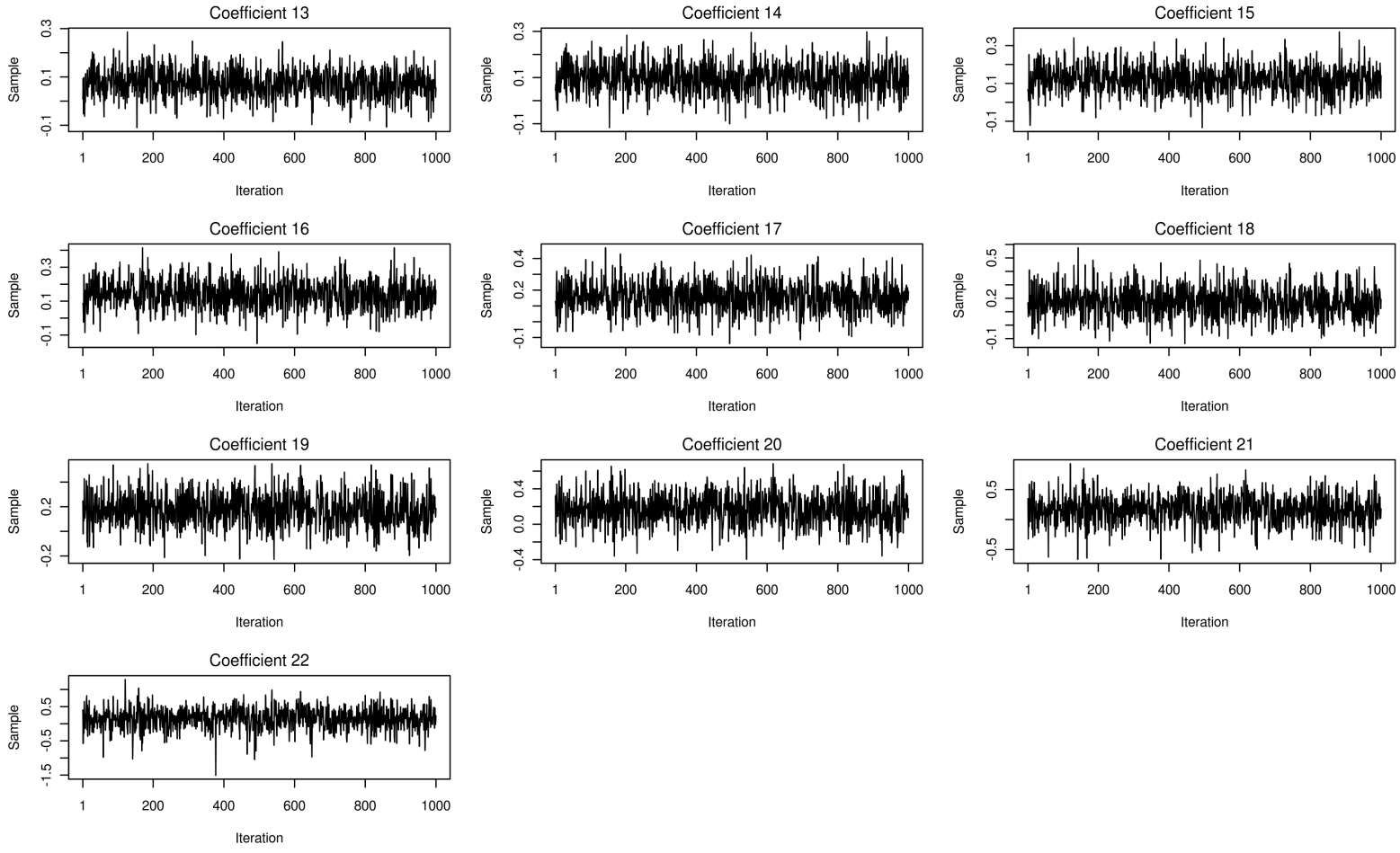
```
R> plot(zm, term = "sx(district)", map = ZambiaBnd)
R> range <- c(-0.32, 0.32)
R> plot(zm, term = "r(district)", map = ZambiaBnd, range = range,
+     lrange = range)
```



# Illustration

## Diagnostic plots, sampling paths

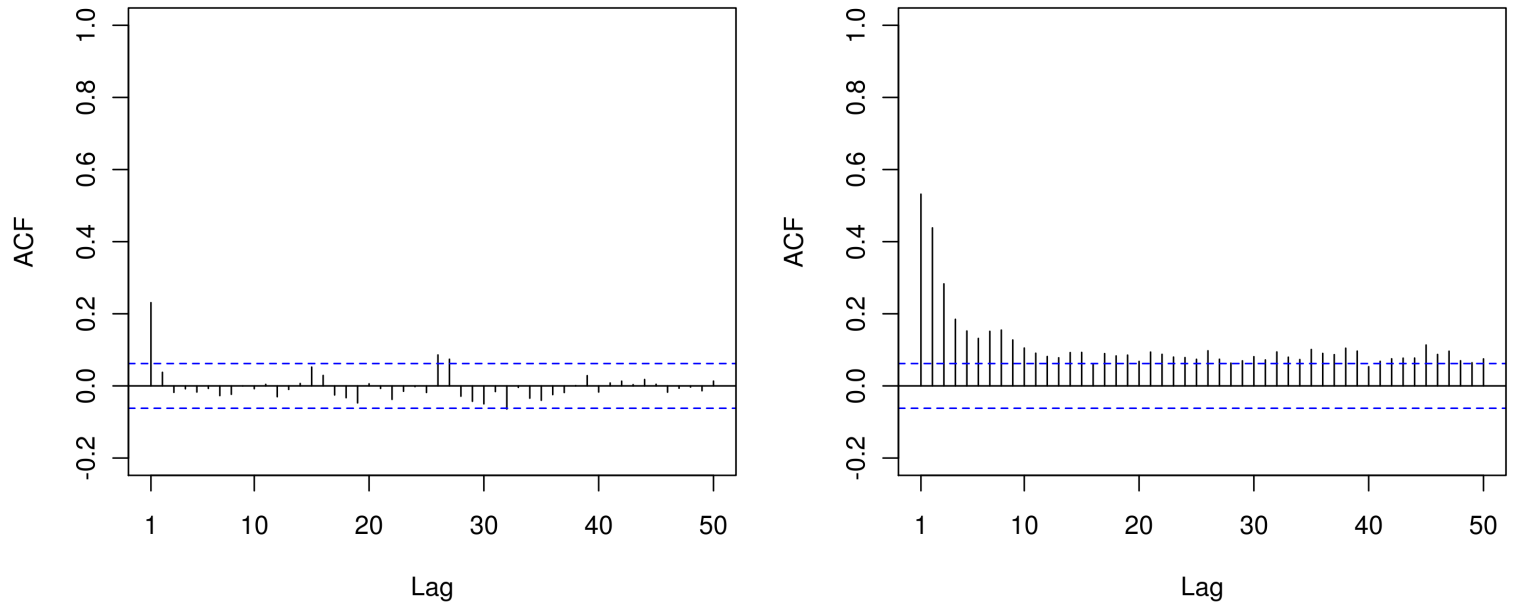
```
R> plot(zm, term = "sx(mbmi)", which = "coef-samples")
```



# Illustration

Diagnostic plots, autocorrelation functions and maximum autocorrelation of parameters

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




Further inspection through extractor function `samples()`, e.g. with package **coda** is possible.

# Illustration

Inspecting the log-file of the **BayesX** binary

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

```
> bayesreg b
> 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=2052766222 predict using d
      .
      .
      .
```

# Outlook

- Beta testing and bug fixing.
- Facilitate installation of **BayesX** binary across platforms.
- Release the package through CRAN.
- Enhance functionality of the package, i.e. support spatial objects (e.g. from **sp**), more options for visualization etc.

The slides together with a package vignette, the R code and demos are available at:

`http://bayesr.R-Forge.R-project.org/`

# References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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.

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