bamlss: A Lego Toolbox for Flexible Bayesian Regression (and Beyond)

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Abstract

Over the last decades, the challenges in applied regression and in predictive modeling have been changing considerably: (1) More flexible model specifications are needed as big(ger) data become available, facilitated by more powerful computing infrastructure. (2) Full probabilistic modeling rather than predicting just means or expectations is crucial in many applications. (3) Interest in Bayesian inference has been increasing both as an appealing framework for regularizing or penalizing model estimation as well as a natural alternative to classical frequentist inference. However, while there has been a lot of research in all three areas, also leading to associated software packages, a modular software implementation that allows to easily combine all three aspects has not yet been available. For filling this gap, the R package bamlss is introduced for Bayesian additive models for location, scale, and shape (and beyond). At the core of the package are algorithms for highly-efficient Bayesian estimation and inference that can be applied to generalized additive models (GAMs) or generalized additive models for location, scale, and shape (GAMLSS), also known as distributional regression. However, its building blocks are designed as “Lego bricks” encompassing various distributions (exponential family, Cox, joint models, ...), regression terms (linear, splines, random effects, tensor products, spatial fields, ...), and estimators (MCMC, backfitting, gradient boosting, lasso, ...). It is demonstrated how these can be easily recombined to make classical models more flexible or create new custom models for specific modeling challenges.

Keywords: GAMLSS, distributional regression, probabilistic forecasting, backfitting, gradient boosting, lasso, MCMC, R.

1. Introduction

Many modern modeling tasks necessitate flexible regression tools that can deal with: (1) Big data sets that can be both long (many observations) and/or wide (many variables or complex effect types). (2) Probabilistic forecasts that capture the entire distribution and not only its mean or expectation. (3) Enhanced inference infrastructure, typically Bayesian, beyond classical frequentist significance tests. A popular framework to combine flexible regression with probabilistic modeling are generalized additive models (GAMs, Hastie and Tibshirani 1990), later extended to generalized additive models for location, scale, and shape (GAMLSS, Rigby and Stasinopoulos 2005), also known as distributional regression (Klein, Kneib, Lang, and Sohn 2015c) which encompasses basic (generalized) linear models (Nelder and Wedderburn 1972) as special cases. These regression approaches can also be combined with Bayesian
inference (see e.g., Fahrmeir, Kneib, Lang, and Marx 2013) as a natural framework for penalizing flexible model terms and to overcome potential problems with $p$ values and classical null hypothesis significance testing (Wasserstein and Lazar 2016). However, when fitting such models to big data – long and/or wide – classical estimation techniques using standard algorithms like iteratively weighted least squares (IWLS) or Markov chain Monte Carlo (MCMC) might not be feasible. Instead, regularized estimation techniques such as lasso or boosting (Friedman, Hastie, and Tibshirani 2010; Mayr, Fenske, Hofner, Kneib, and Schmid 2012) might be necessary or custom algorithms (Wood 2017). Hence, to facilitate combining all three aspects discussed above with different estimation techniques and fitting algorithms, the bamlss package for the R system for statistical computing (R Core Team 2019) implements a modular “Lego toolbox”, extending the work of Umlauf, Klein, and Zeileis (2018). In this framework not only the response distribution or the regression terms are “Lego bricks” but also the estimation algorithm or the MCMC sampler.

In terms of software infrastructure, the R ecosystem already provides a rich variety of packages that combine several – but not all – of the aspects discussed above.

- **GAMs and GAMLSSs** are available in a number of packages, most notably the mgcv package (Wood 2017) and also the gamlss family of packages (Stasinopoulos and Rigby 2007) and VGAM (Yee 2010). The latter two are notable for their support of a wide range of response distributions. However, for complex predictor structures and response distributions beyond the exponential family, estimation may be challenging or subject to numerical instabilities. In contrast, mgcv excels at providing highly-optimized algorithms for general smooth models (Wood, Pya, and Säfken 2016) as well as the dedicated bam() function for big data that is long and/or wide (Wood, Li, Shaddick, and Augustin 2017).

- **Bayesian inference** is not only an increasingly popular alternative to classical frequentist inference, it is also particularly attractive for hierarchical or multilevel models and for penalizing regression effects through suitable prior distributions. Also, fully Bayesian approaches using MCMC are appealing in flexible regression models for obtaining credible intervals from the posterior samples etc. The brms package (Bürkner 2017) is notable for providing a standard R workflow for estimating Bayesian multilevel models using Stan (Carpenter, Gelman, Hoffman, Lee, Goodrich, Betancourt, Brubaker, Guo, Li, and Riddell 2017). Also, the above-mentioned mgcv package supports estimation of Bayesian GAMs via its jagam() function (Wood 2016) based on JAGS (Plummer 2003).

For more flexibility, going beyond these capabilities, it is in principle possible to directly implement custom models using general purpose MCMC software like JAGS, Stan, or WinBUGS (Lunn, Thomas, Best, and Spiegelhalter 2000). However, for complex models – e.g., using large data sets, spatial effects, or higher-order interactions – sampling times from these generic MCMC engines can become long, sometimes prohibitively so. This has been addressed by dedicated packages for Bayesian additive models, e.g., with the standalone package BayesX (Brezger, Kneib, and Lang 2005) being the first to provide highly-efficient sampling schemes for very large data sets as well as spatial/multilevel models. An R interface is available in R2BayesX (Umlauf, Adler, Kneib, Lang, and Zeileis 2015). Instead of fully Bayesian MCMC it is also possible to employ posterior mean estimation via the integrated nested Laplace approximation to estimate flexible
Bayesian regression models. This is provided in the comprehensive R package INLA (Rue, Martino, and Chopin 2009), popular for estimating complex spatial Bayesian regression models (see e.g., Lindgren and Rue 2015; Bivand, Gómez-Rubio, and Rue 2015).

- **Regularized estimation** might be necessary, though, for going beyond the models described above, especially for large/wide data with many potential regressors and corresponding effects/interactions/etc. Widely-used approaches for this include the lasso, e.g., as available for GLM-type models in the R package glmnet (Friedman et al. 2010), or gradient boosting as available for GAMLSS-type models in the R package gamboostLSS (Hofner, Mayr, and Schmid 2016). However, obtaining MCMC samples from the posterior distributions corresponding to such models is not easily available in these packages.

In summary, the discussion above highlights that many different packages with different strengths are already available in R. However, a package combining all the aspects above in a single framework is not readily available as there are typically limitations with respect to the inferential framework, the distributions and/or complexity of the models supported, or the estimation techniques and fitting algorithms. The package bamlss, available from the Comprehensive R Archive Network at https://CRAN.R-project.org/package=bamlss, tries to fill this gap with a modular “Lego” approach to flexible Bayesian regression providing:

- The usual R “look & feel” for regression modeling.
- Estimation of classic (GAM-type) regression models (Bayesian or frequentist).
- Estimation of flexible (GAMLSS-type) distributional regression models.
- An extensible “plug & play” approach for regression terms.
- Modular combinations of fitting algorithms and samplers.

Especially the last item is notable because the models in bamlss are not limited to a specific estimation algorithm but different engines can be plugged in without necessitating changes in other aspects of the model specification (such as response distributions or regression terms). By default bamlss is using IWLS-based backfitting for optimizing the model and IWLS-based MCMC for sampling from the posterior distribution. However, alternative optimizers and samplers are also implemented that support lasso or boosting etc. Moreover, the package builds on the well-established mgcv infrastructure for smooth model terms, uses R’s formula syntax for model specification, and provides standard extractor methods like summary(), plot(), predict(), etc.

The remainder of this paper is as follows. In Section 2, three motivating examples illustrate the first steps using bamlss and show cases the flexibility of the provided infrastructures. Section 3 introduces the flexible regression framework in more detail. A thorough introduction of the R package bamlss, describing the most important building blocks for developing families, model terms and estimation algorithms, is then given in Section 4. In Section 5 we highlight the unified modeling approach using a complex distributional regression model for lighting counts in complex terrain. Further details and examples about the bamlss package can be found online at http://www.bamlss.org/.
2. Motivating examples

This section gives a first quick overview of the functionality of the package. The first example demonstrates that the usual “look & feel” when using well-established model fitting functions like `glm()` is an elementary part of `bamlss`, i.e., first steps and basic handling of the package should be relatively simple. The second example shows that the package can deal with a variety of different model terms and that model fitting functions can easily be exchanged, here, we exemplify this feature by applying a lasso-type estimation engine. The third example then explains how full distributional regression models can be estimated and show cases once more the flexibility of the provided modeling infrastructures.

2.1. Basic Bayesian regression: Logit model

This example data is taken from the AER package (Kleiber and Zeileis 2008) and is about labor force participation (yes/no) of women in Switzerland 1981 (Gerfin 1996). The `bamlss` package and the data can be loaded with

```r
R> library("bamlss")
R> data("SwissLabor", package = "AER")
```

The data frame contains 872 observations of 6 variables, where some of them might have a nonlinear influence on the response labor participation. Now, a standard Bayesian binomial logit model using the default MCMC algorithm can be fitted. First, the model formula specified with

```r
R> f <- participation ~ income + age + education +
+   youngkids + oldkids + foreign + I(age^2)
```

Then, to reproduce the results the seed of the random number generator is set to

```r
R> set.seed(123)
```

The model is estimated by

```r
R> b <- bamlss(f, family = "binomial", data = SwissLabor)
```

Note that the default number of iterations for the MCMC sampler is 1200, the burnin-phase is 200 and thinning is 1. The reason is that during the modeling process, users usually want to obtain first results rather quickly. Afterwards, if a final model is estimated the number of iterations of the sampler is usually set much higher to get close to i.i.d. samples from the posterior distribution. To obtain reasonable starting values for the MCMC sampler we run a backfitting algorithm that optimizes the posterior mode. Using the main model fitting function `bamlss()` all model fitting engines can be exchanged, which is explained in detail in Section 4 and the application Section 5. The default model fitting engines use family objects (see also Section 4), similar to the families that can be used with the `glm()` function, which enables easy implementation of new distributions (models).

Note, to capture nonlinearities, a quadratic term for variable `age` is added to the model. The resulting object `b` is of class "bamlss" for which standard extractor functions like `summary()`, `coef()`, `plot()`, `predict()`, etc. are available. The model summary output is printed by
R> summary(b)

Call:
bamlss(formula = f, family = "binomial", data = SwissLabor)

---
Family: binomial
Link function: pi = logit
---
Formula pi:

participation ~ income + age + education + youngkids + oldkids + 
   foreign + I(age^2)

---
Parametric coefficients:

| Parameter     | Mean     | 2.5%     | 50%      | 97.5%    | 97.5% parameters |
|---------------|----------|----------|----------|----------|------------------|
| (Intercept)   | 6.15503  | 1.55586  | 5.99204  | 11.11051 | 6.196            |
| income        | -1.10565 | -1.56986 | -1.10784 | -0.68652 | -1.104           |
| age           | 3.45703  | 2.05897  | 3.44567  | 4.79139  | 3.437            |
| education     | 0.03354  | -0.02175 | 0.03284  | 0.09223  | 0.033            |
| youngkids     | -1.17906 | -1.51099 | -1.17683 | -0.83047 | -1.186           |
| oldkids       | -0.24122 | -0.41231 | -0.24099 | -0.08054 | -0.241           |
| foreignyes    | 1.16749  | 0.76276  | 1.17035  | 1.55624  | 1.168            |
| I(age^2)      | -0.48990 | -0.65660 | -0.49205 | -0.31968 | -0.488           |
| alpha         | 0.87585  | 0.32301  | 0.99408  | 1.00000  | NA               |

---
Sampler summary:

DIC = 1033.325 logLik = -512.7258 pd = 7.8734
runtime = 1.417
---
Optimizer summary:

AICc = 1033.737 converged = 1 edf = 8
logLik = -508.7851 logPost = -571.3986 nobs = 872
runtime = 0.012
---

and is based on MCMC samples, which suggest “significant” effects for all covariates, except for variable education, since the 95% credible interval contains zero. In addition, the acceptance probabilities alpha are reported and indicate proper behavior of the MCMC algorithm. The column parameters shows respective posterior mode estimates of the regression coefficients, which are calculated by the upstream backfitting algorithm. Before proceeding the analysis, users usually perform additional convergence checks of the MCMC chains by looking at traceplots and auto-correlation.

R> plot(b, which = c("samples", "max-acf"))
Figure 1: Logit model, MCMC trace (left panel), auto-correlation for the intercept (middle panel), maximum auto-correlation for all parameters (right panel).

These are visualized in Figure 1 and reveal approximate convergence of the MCMC chains, i.e., there is no visible trend and the very low auto-correlation shown for the intercept and the maximum auto-correlation of all parameters suggest close to i.i.d. samples from the posterior distribution. As mentioned above, the user could also increase the number iterations and the burnin-phase, as well as adapt the thinning parameter, to make the significant bar at lag one disappear. Note that the function call would compute all trace- and auto-correlation plots, however, for convenience we only show plots for the intercept. In addition, samples can also be extracted using function `samples()`, which returns an object of class "mcmc", a class provided by the `coda` package (Plummer, Best, Cowles, and Vines 2006). This package includes a rich infrastructure for further convergence diagnostic checks, e.g., Gelman and Rubin’s convergence diagnostic (Gelman and Rubin 1992; Brooks and Gelman 1998) or Heidelberger and Welch’s convergence diagnostic (Heidelberger and Welch 1981, 1983).

Model predictions on the probability scale can be obtained by the predict method, e.g., to visualize the effect of covariate `age` on the probability we can create a new data frame for prediction

```R
nd <- data.frame(income = 11, age = seq(2, 6.2, length = 100),
+ education = 12, youngkids = 1, oldkids = 1, foreign = "no")
```

Afterwards, we predict for both cases of variable `foreign`

```R
R> nd$pSwiss <- predict(b, newdata = nd, type = "parameter", FUN = c95)
R> nd$foreign <- "yes"
R> nd$pForeign <- predict(b, newdata = nd, type = "parameter", FUN = c95)
```

The predict method is applied on all MCMC samples and argument `FUN` specifies a function that can be applied on the predictor or distribution parameter samples. The default is the `mean()` function, however, in this case we additionally extract the empirical 2.5% and 97.5% quantiles using function `c95()` to obtain credible intervals (note, individual samples can be extracted by passing `FUN = identity`, i.e., this way users can easily generate their own statistics). Then, the estimated effect can be visualized with
Figure 2: Left panel, quadratic polynomial effect of covariate age on estimated probabilities for both cases, foreign "yes" and "no". Right panel, effect on Logit$^{-1}(\pi)$ of variable age using regression splines (see Section 2.2). The solid lines represent mean estimates, the shaded areas show 95% credible intervals.

\begin{verbatim}
R> blues <- function(n, ...) sequential_hcl(n, "Blues", rev = TRUE)
R> plot2d(pSwiss ~ age, data = nd, ylab = "participation",
+       ylim = range(c(nd$pSwiss, nd$pForeign)),
+       fill.select = c(0, 1, 0, 1))
R> plot2d(pForeign ~ age, data = nd, add = TRUE,
+       fill.select = c(0, 1, 0, 1), axes = FALSE,
+       s2.col = blues, col.lines = blues(1))
\end{verbatim}

The estimates are shown in Figure 2 and suggest a clear difference for the effect of age between both cases of factor variable foreign.

2.2. Flexible model terms and estimators

Using the flexible infrastructure of bamlss, model terms can be easily exchanged. To give a first impression of the modeling capabilities, we again use the SwissLabor data and binomial logit model of Section 2.1, however, in this example we use regression splines to capture the nonlinear effect variable age.

As noted in the introduction, the bamlss package heavily builds upon the R package mgcv (Wood 2019) infrastructures. To estimate a spline model instead of a polynomial model for variable age the model formula only needs to be slightly adapted

\begin{verbatim}
R> f <- participation ~ income + education +
+       youngkids + oldkids + foreign + s(age, k = 10)
\end{verbatim}

The function s() is the smooth term constructor from the mgcv package, the default of s() are thin-plate regression splines with $k = 10$ basis functions. The model is again fitted by

\begin{verbatim}
R> set.seed(123)
R> b <- bamlss(f, family = "binomial", data = SwissLabor)
\end{verbatim}

The estimated nonlinear effect can be plotted instantly by typing
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| Description | Formula |
|-------------|---------|
| Linear effects: $X\beta$ | $x_1 + x_2 + x_3$ |
| Nonlinear effects of continuous covariates: $f(x) = f(x_1)$ | $s(x_1)$ |
| Two-dimensional surfaces: $f(x) = f(x_1, x_2)$ | $s(x_1,x_2), te(x_1,x_2)$ or $ti(x_1,x_2)$ (higher dimensional terms possible). |
| Spatially correlated effects: $f(x) = f_{\text{spat}}(x)$ | $s(xs, bs = "mrf", xt = \text{list(penalty = K)}), where xs is a factor indicating the discrete regional information and K is a supplied penalty matrix. Other options within the xt argument are possible, please see the documentation of smooth.construct.mrf.smooth.spec(). |
| Varying coefficients: $f(x) = x_1f(x_2)$ | $s(x_2, by = x_1)$ |
| Spatially varying effects: $f(x) = x_1f_{\text{spat}}(x)$ or $f(x) = x_1f(x_2, x_3)$ | $s(xs, bs = "mrf", xt = \text{list(penalty = K)}, by = x_1), s(x_2, x_3, by = x_1)$ or $te(x_2, x_3, by = x_1)$ |
| Random intercepts with cluster index $c$: $f(x) = \beta_c$ | $s(id, bs = "re"), where id is a factor of cluster indices. |
| Random slopes with cluster index $c$: $f(x) = x_1\beta_c$ | $s(id, x_1, bs = "re"), as above with continuous covariate x_1. |

Table 1: Commonly used model term specifications with respective R formula syntax.

```r
R> plot(b, term = "s(age)")
```

The estimated effect based on regression splines is shown in the right panel of Figure 2 and reveals that the quadratic polynomial seems to capture the nonlinearity appropriately.

To give a better impression what type of model terms can be used with the bamlss framework Table 1 lists commonly used specifications.

Besides the supported infrastructures from the mgcv package, it is also possible to implement completely new model terms that may follow different setups compared to the basis functions approach (see also Appendix C for an example using growth curves). Moreover, using bamlss, estimation engines can also be exchanged. To give an example we estimate the nonlinear age effect in the SwissLabor example using a fused lasso algorithm (see also Section 5 for a complex example using gradient boosting optimization). The algorithm performs variable selection in combination with factor fusion (clustering) and can also be used to identify interpretable nonlinearities. Methodological details on lasso-type penalization using bamlss are provided in Groll, Hambuckers, Kneib, and Umlauf (2019). To apply the fused lasso, the numeric variable age is categorized using empirical quantiles, e.g., with

```r
R> SwissLabor<cage <- cut(SwissLabor$age, + breaks = quantile(SwissLabor$age, prob = seq(0, 1, length = 10)), + include.lowest = TRUE, ordered_result = TRUE)
```

The formula for the fused lasso model is then specified with the special `la()` model term constructor function provided in bamlss:
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Figure 3: Left panel, BIC curve with optimum shrinkage parameter $\lambda$ of the lasso example model. The middle panel shows the corresponding coefficient paths for variable \textit{cage}. The right panel displays the respective estimated effect.

\begin{verbatim}
R> f <- participation ~ income + education + youngkids + oldkids + foreign + + la(cage, fuse = 2)
\end{verbatim}

where argument \texttt{fuse} specifies the type of fusion (nominal fusion \texttt{fuse = 1}, ordered fusion \texttt{fuse = 2}). To estimate the fused lasso model only the default \texttt{optimizer} function in the \texttt{bamlss()} wrapper function call needs to exchanged

\begin{verbatim}
R> b <- bamlss(f, family = "binomial", data = SwissLabor, + optimizer = lasso, sampler = FALSE, + criterion = "BIC", upper = exp(5), lower = 1)
\end{verbatim}

The optimum shrinkage parameter $\lambda$ is selected by the BIC. Arguments \texttt{upper} and \texttt{lower} determine the search interval of $\lambda$, per default \texttt{nlambda = 100} values are generated. Note that no MCMC sampling is used after the \texttt{lasso()} estimation engine is applied, argument \texttt{sampler = FALSE} in the \texttt{bamlss()} call.

The BIC curve and the coefficient paths including the optimum shrinkage parameter $\lambda$ can be visualized with

\begin{verbatim}
R> pathplot(b)
\end{verbatim}

Figure 3 shows the BIC curve and coefficient paths for \textit{cage}. The BIC curve assumes a clear minimum at the vertical gray dashed line. The coefficient paths obviously depict that the algorithm can either shrink categories out of the model (shrink to zero), or even fuses them. In the right panel of Figure 3, the estimated effect of the categorized variable \textit{age} is shown. The effect is computed by predicting without intercept using the optimum stopping iteration, which is selected by BIC and can be extracted with function \texttt{lasso_stop()}. The stopping iteration is passed to the \texttt{predict()} method by specifying the \texttt{mstop} argument.

\begin{verbatim}
R> page <- predict(b, term = "cage", intercept = FALSE, + mstop = lasso_stop(b))
\end{verbatim}
The figure is then created using the untransformed original covariate on the x-axis.

R> plot2d(page ~ age, data = SwissLabor, rug = TRUE)

Using the fused lasso estimation some nonlinearities can be identified again, however, the BIC criterion seems to shrink out the positive effects that are shown for the spline estimate in the right panel of Figure 2.

2.3. Location-scale model

In this example we will now extend the framework and estimate a complete distributional regression model using a small textbook example of the well-known simulated motorcycle accident data (Silverman 1985).

R> data("mcycle", package = "MASS")

The data set contains measurements of the head acceleration (in g, variable accel) in a simulated motorcycle accident, recorded in milliseconds after impact (variable times). To estimate a location-scale model with

\[ \text{accel} \sim \mathcal{N}(\mu = f_\mu(\text{times}), \log(\sigma) = f_\sigma(\text{times})) \]

where functions \(f_\mu(\cdot)\) and \(f_\sigma(\cdot)\) are unspecified smooth functions, which are estimated using regression splines. The log-link for parameter \(\sigma\) ensures positivity. We can use the following model formula for estimation

R> f <- list(accel ~ s(times, k = 20), sigma ~ s(times, k = 20))

again, function \(s()\) is the smooth term constructor from the \texttt{mgcv} package (Wood 2019). Note that model formulae are provided as lists of formulae, i.e., each list entry represents one parameter of the response distribution. Moreover, note that all smooth terms, i.e., \texttt{te()}, \texttt{ti()}, etc., are supported by \texttt{bamlss}. This way, it is also possible to incorporate user defined model terms. A full Bayesian semi-parametric distributional regression model can be estimated with

R> set.seed(456)
R> b <- bamlss(f, family = "gaussian", data = mcycle)

After the estimation algorithms are finished, the estimated effects can be visualized instantly using the plotting method.

R> plot(b, model = c("mu", "sigma"))

The estimated effects are shown in Figure 4 depicting a clear nonlinear relationship for parameter \(\mu\) and \(\sigma\).

For judging how well the model fits to the data the user can inspect randomized quantile residuals (Dunn and Smyth 1996) using histograms or quantile-quantile plots. Residuals can be extracted using function \texttt{residuals()} and has a plotting method. Alternatively, residuals can be investigated with
Figure 4: Estimated effects of times on parameter $\mu$ and $\sigma$ of the normal location-scale model. The grey shaded areas represent 95% credible intervals.

Figure 5: Histogram and quantile-quantile plot of the resulting randomized quantile residuals of the normal location-scale model.

\begin{verbatim}
R> plot(b, which = c("hist-resid", "qq-resid"))
\end{verbatim}

According to the histogram and the quantile-quantile plot of the resulting randomized quantile residuals in Figure 5, the model seems to fit relatively well. Only for very low and very high values of $\text{accel}$ the fitted distributions seem to be less appropriate.

Besides residuals, users can evaluate the model performance, e.g., for model selection based on the deviance information criterion (DIC), which can be extracted using function `DIC()`

\begin{verbatim}
R> DIC(b)
\end{verbatim}

\begin{verbatim}
DIC pd
1115.247 24.07131
\end{verbatim}

and is also reported in the model summary output. Furthermore, statistical calibration of fitted models can be assessed by scoring rules (Gneiting and Raftery 2007; Gneiting, Balab-)
3. A flexible Bayesian model framework

This section briefly summarizes the BAMLSS modeling framework. For a detailed methodological description please refer to Umlauf et al. (2018), as well as to the references given below on page 13 that discuss various applications and extensions that are also implemented in bamlss. The following outlines the framework from the viewpoint of distributional regression models, however, please note that model classes like, e.g., GLMs and GAMs or even survival joint models (Köhler, Umlauf, Beyerlein, Winkler, Ziegler, and Greven 2017; Köhler, Umlauf, and Greven 2018) are special cases in this setup.

3.1. Model structure

Within the framework of GAMLSS or distributional regression models all parameters of the response distribution can be modeled by explanatory variables such that

\[
y \sim D(h_1(\theta_1) = \eta_1, \ h_2(\theta_2) = \eta_2, \ldots, \ h_K(\theta_K) = \eta_K),
\]

where \(D\) denotes a parametric distribution for the response variable \(y\) with \(K\) parameters \(\theta_k, k = 1, \ldots, K\), that are linked to additive predictors using known monotonic and twice differentiable functions \(h_k(\cdot)\). Note that the response may also be a \(q\)-dimensional vector \(y = (y_1, \ldots, y_q)^\top\), e.g., when \(D\) is a multivariate distribution (see, e.g., Klein, Kneib, Klasen, and Lang 2015a). The additive predictor for the \(k\)-th parameter is given by

\[
\eta_k = \eta_k(X; \beta_k) = f_{1k}(X; \beta_{1k}) + \ldots + f_{Jk}(X; \beta_{Jk}),
\]

based on \(j = 1, \ldots, J_k\) unspecified (possibly nonlinear) functions \(f_{jk}(\cdot)\), applied to each row of the generic data matrix \(X\), encompassing all available covariate information. The corresponding parameters \(\beta_k = (\beta_{1k}, \ldots, \beta_{Jk})^\top\) are typically regression coefficients pertaining to model matrices \(X_k = (X_{1k}, \ldots, X_{Jk})^\top\), whose structure only depend on the type of covariate(s) and prior assumptions about \(f_{jk}(\cdot)\).

Usually, functions \(f_{jk}(\cdot)\) are based on a basis function approach, where \(\eta_k\) then is a typical GAM-type or so-called structured additive predictor (STAR, Fahrmeir, Kneib, and Lang 2004). Umlauf et al. (2018) relax this assumption and let \(f_{jk}(\cdot)\) be an unspecified composition of covariate data and regression coefficients. For example, functions \(f_{jk}(\cdot)\) could also represent nonlinear growth curves, a regression tree, a neural network or lasso-penalized model terms as shown in Section 2.2.

For full Bayesian inference, priors need to be assigned to the regression coefficients \(\beta_{jk}\). To be as flexible as possible, Umlauf et al. (2018) use the rather general prior \(p_{jk}(\beta_{jk}; \tau_{jk}, \alpha_{jk})\) for the \(j\)-th model term of the \(k\)-th parameter, where the form of \(p_{jk}(\cdot)\) depends on the type of function \(f_{jk}(\cdot)\). Here, \(\tau = (\tau_{11}, \ldots, \tau_{1K}, \ldots, \tau_{J1}, \ldots, \tau_{JK})^\top\) is the vector of all assigned hyper-parameters, e.g., representing smoothing variances (shrinkage parameters). Similarly, \(\alpha_{jk}\) is the set of all prior specifications. In most situations the prior \(p_{jk}(\beta_{jk}; \tau_{jk}, \alpha_{jk})\) is
based on a multivariate normal kernel for $\beta_{jk}$ and on inverse gamma distributions for each $\tau_{jk} = (\tau_{1jk}, \ldots, \tau_{Ljk})^T$, but as indicated previously, in principle any type of prior can be used (see Gelman 2006; Polson and Scott 2012; Klein and Kneib 2016a; Umlauf et al. 2018 for more detailed discussions on priors for $\beta_{jk}$ and $\tau_{jk}$).

Examples of distributional models that fit well in this framework are the ones for:

- Univariate responses of any type, e.g. counts with zero-inflation and or overdispersion as proposed in Klein, Kneib, and Lang (2015b); Herwartz, Klein, and Strumann (2016), continuous responses with spikes, skewness, heavy tails or bounded support as in Klein et al. (2015c); Klein, Denuit, Lang, and Kneib (2014), as well as responses for extreme events (Umlauf and Kneib 2018).
- Multivariate responses such as multivariate normal, multivariate t or Dirichlet regression (for analyzing compositional data, Klein et al. 2015a).
- Multivariate responses with more complex dependence structures modeled through copulas Klein and Kneib (2016b).
- Survival data and joint modeling (Köhler et al. 2017; Köhler et al. 2018).

### 3.2. Posterior estimation

Estimation typically requires to evaluate the log-likelihood $\ell(\beta; y, X)$ function and its derivatives w.r.t. all regression coefficients $\beta$ a number of times. For fully Bayesian inference the log-posterior is either used for posterior mode estimation, or for solving high-dimensional integrals. e.g., for posterior mean estimation MCMC samples need to be computed.

Although the types of models that can be fitted within the flexible BAMLSS framework can be quite complex, Umlauf et al. (2018) show that there are a number of similarities between optimization and sampling concepts. Fortunately, and albeit the different model term complexity, algorithms for posterior mode and mean estimation can be summarized into a partitioned updating scheme with separate updating equations using leapfrog or zigzag iteration (Smyth 1996), e.g., with updating equations

$$
(\beta_{jk}^{(t+1)}, \tau_{jk}^{(t+1)}) = U_{jk}(\beta_{jk}^{(t)}, \tau_{jk}^{(t)}; \cdot) \quad j = 1, \ldots, J_k, \quad k = 1, \ldots, K,
$$

where function $U_{jk}(\cdot)$ is an updating function, e.g., for generating one Newton-Raphson step or for getting the next step in an MCMC simulation, a.o.

Using a basis function approach, the updating functions $U_{jk}(\cdot)$ for posterior mode (frequentist penalized likelihood) estimation or MCMC for $\beta_{jk}$ share an iteratively weighted least squares updating step (IWLS, Gamerman 1997)

$$
\beta_{jk}^{(t+1)} = U_{jk}(\beta_{jk}^{(t)}; \cdot) = (X_{jk}^T W_{kk} X_{jk} + G_{jk}^\tau(\tau_{jk}))^{-1} X_{jk}^T W_{kk} (z_k - \eta_{k, \cdot}^{(t+1)}),
$$

with weight matrices $W_{kk}$ and working responses $z_k$, similarly to the well-known IWLS updating scheme for generalized linear models (GLM, Nelder and Wedderburn 1972). The matrices $G_{jk}^\tau(\tau_{jk})$ are derivative matrices of the priors $p_{jk}(\beta_{jk}; \tau_{jk}, \alpha_{jk})$ w.r.t. the regression coefficients $\beta_{jk}$, e.g., $G_{jk}^\tau(\tau_{jk})$ can be a penalty matrices that penalizes the complexity of $f_{jk}(\cdot)$ using a P-spline representation (Eilers and Marx 1996).
Even if the functions $f_{jk}(\cdot)$ are not based on a basis function approach, the updating scheme (4) can be further generalized to

$$\beta_{jk}^{(t+1)} = U_{jk} \left( \beta_{jk}^{(t)}, z_k - \eta_{k,-j}^{(t+1)}, \cdot \right),$$

i.e., theoretically any updating function applied to the “partial residuals” $z_k - \eta_{k,-j}^{(t+1)}$ can be used. (For detailed derivations see Umlauf et al. 2018.)

The great advantage of this modular architecture is, that the concept does not limit to modeling of the distributional parameters $\theta_k$ in (1), e.g. as mentioned above, based on the survival function, Köhler et al. (2017) and Köhler et al. (2018) implement Bayesian joint models for survival and longitudinal data. Moreover, the updating schemes do not restrict to any particular estimation engine, e.g., Groll et al. (2019) use the framework to implement lasso-type penalization for GAMLSS and Simon, Fabsic, Mayr, Umlauf, and Zeileis (2018) investigate gradient boosting with stability selection algorithms (see also Section 5). Very recently, Klein, Simon, and Umlauf (2019) implement neural network distributional regression models.

3.3. Model choice and evaluation

**Measures of performance**

Model choice and variable selection is important in distributional regression due to the large number of candidate models. The following lists commonly used tools:

- **Information criteria** can be used to compare different model specifications. For posterior mode estimation, the Akaike information criterion (AIC), or the corrected AIC, as well as the Bayesian information criterion (BIC), can be used. Estimation of model complexity is based on the so-called equivalent degrees of freedom (EDF).
  
  For MCMC based estimation, model choice mainly relies on the deviance information criterion (DIC, Spiegelhalter, Best, Carlin, and Van Der Linde 2002) and the widely applicable information criterion (WAIC, Watanabe 2010).

- **Quantile residuals** (Dunn and Smyth 1996) can be used to evaluate the model fit. The residuals can be assessed by quantile-quantile-plots, probability integral transforms (PIT) histograms (Gneiting et al. 2007) or worm plots (Van Buuren and Fredriks 2001).

- **Scoring rules**: Sometimes it is helpful to evaluate the performance on a test data set (or for instance based on cross validation). For this, proper scoring rules (Gneiting and Raftery 2007; Gneiting et al. 2007) can be utilized.

**Evaluation and interpretation**

- **Plotting**: Estimated functions $\hat{f}_{jk}(\cdot)$ are usually centered around their mean, therefore, simple effect plots are a straightforward method to evaluate individual model term importance and can also be used for respective interpretations. Sometimes it can be useful in distributional regression to look at transformations of the original model parameters such as expected value or variance of the response variable $y$. 

• **Predictions**: For obtaining such transformations model predictions need to be computed. This can be done either manually by the corresponding `predict()` method, or by the R package `distreg.vis` (Stadlmann 2019), which provides a graphical user interface for visualization of distributional regression models.

4. **The bamlss package**

The R package `bamlss` provides a modular software architecture for flexible Bayesian regression models (and beyond). The implementation follows the conceptional framework presented in Umlauf et al. (2018), which supports Bayesian and/or frequentist estimation engines using complex possibly nonlinear model terms of any type. The highlights of the package are:

- A unified model description where a *formula* specifies how to set up the predictors from the *data* and the *family*, which holds information about the response distribution, the model.

- A generic method for setting up model terms and a `model.frame()` for BAMLSS, the `bamlss.frame()`, along with the corresponding prior structures. A `transform()` function can optionally set up modified terms, e.g., using mixed model representation for smooth terms.

- Support for modular and exchangeable updating functions or complete model fitting engines in order to optionally implement either algorithms for maximization of the log-posterior for posterior mode estimation or for solving high-dimensional integrals, e.g., for posterior mean or median estimation. First, an (optional) `optimizer()` function can be run, e.g., for computing posterior mode estimates. Second, a `sampler()` is employed for full Bayesian inference with MCMC, which uses the posterior mode estimates from the `optimizer()` as staring values. An additional step can be used for preparing the `results()`, e.g., for creating model term effect plots.

- Standard post-modeling extractor functions to create sampling statistics, visualizations, predictions, etc.

The modular architecture of `bamlss` is illustrated in Figure 6. As mentioned above, the first step in model development is to setup design and penalty matrices for a model that is specified by the *family* object. Therefore a *formula* is processed together with the *data* using the `bamlss.frame()` function. In a second pre-processing step, the returned model frame may also be transformed. The BAMLSS model frame can then be used with `optimizer()` and/or `sampler()` functions in the estimation step. This is probably the main advantage of the architecture, users can easily exchange and integrate user defined estimation functions. The only requirement is to keep the structure of the `bamlss.frame()` function, as well for `optimizer()` and `sampler()` functions. After the estimation step optional post-processing functions can be applied to create additional sampling statistics, function `samplestats()`, or results that can be used for plotting the estimated effects, function `results()`. Note that the post-processing step is optional since it is not necessarily needed in the last output step, e.g., for computing predictions. This feature is especially important when using large data sets, because the run time for computing `samplestats()` or `results()` can be quite long.
Figure 6: Flow chart of the \texttt{bamlss} modeling architecture. Thick gray lines represent optional paths, e.g., after building the \texttt{bamlss.frame()} the user can either run an \texttt{optimizer()} function prior running the \texttt{sampler()}, or run the \texttt{sampler()} function directly.

| Step           | Type                  | Function                                |
|----------------|-----------------------|-----------------------------------------|
| Pre-processing | Parser                | \texttt{bamlss.frame()}                 |
|                | Transformer           | \texttt{bamlss.engine.setup()}, \texttt{randomize()}, \texttt{lasso_transform()} |
| Estimation     | Optimizer             | \texttt{bfit()}, \texttt{bbfit()}, \texttt{boost()}, \texttt{lasso()}, \texttt{cox_mode()}, \texttt{jm_mode()} |
|                | Sampler               | \texttt{GMCMC()}, \texttt{BayesX()}, \texttt{JAGS()}, \texttt{cox_mcmc()}, \texttt{jm_mcmc()} |
| Post-processing| Stats & Results       | \texttt{samplestats()}, \texttt{results.bamlss.default()} |

Table 2: Current available functions that can be used for pre-processing, estimation and post-processing within the \texttt{bamlss} framework.
or computations can even lead to memory problems. In summary, the architecture is very flexible such that users interested in implementing new models only need to focus on the estimation step, i.e., write \texttt{optimizer()} or \texttt{sampler()} functions and get all post-processing and extractor functionalities “for free”. This way, prototyping becomes relatively easy, but also the integration/implementation of (new) high-performance estimation engines is facilitated. Table 2 provides an overview of current available functions.

To exemplify the presented “Lego toolbox”, the following R code estimates the logit model using the \texttt{SwissLabor} data presented in Section 2.1. First, the data is loaded and the model formula is specified with

\begin{verbatim}
R> data("SwissLabor", package = "AER")
R> f <- participation ~ income + age + education +
R>        youngkids + oldkids + foreign + I(age^2)
\end{verbatim}

In the second step, the necessary design matrices are constructed using the model frame parser function \texttt{bamlss.frame()}

\begin{verbatim}
R> bf <- bamlss.frame(f, data = SwissLabor, family = "binomial")
\end{verbatim}

Then, posterior mode estimates are obtained by using the implemented backfitting estimation function \texttt{bfit()}

\begin{verbatim}
R> pm <- with(bf, bfit(x, y, family))
\end{verbatim}

The estimated parameters returned from function \texttt{bfit()} can then be used as starting values for the MCMC sampler function \texttt{GMCMC()}

\begin{verbatim}
R> set.seed(123)
R> samps <- with(bf, GMCMC(x, y, family, start = pm$parameters))
\end{verbatim}

Using the parameters samples returned from function \texttt{GMCMC()}, statistics like the DIC are computed using the \texttt{samplestats()} function

\begin{verbatim}
R> stats <- with(bf, samplestats(samps, x, y, family))
R> print(unlist(stats))
\end{verbatim}

\begin{verbatim}
   logLik  DIC     pd
  -512.72579 1033.32501  7.87343
\end{verbatim}

As one can see in the code above, estimation engines have common arguments \texttt{x} (holding the design and penalty matrices), \texttt{y} (the response data) and \texttt{family} (the \texttt{bamlss} family object). For implementing new estimation engines, users only need to keep the argument structures and the return values, i.e., for \texttt{optimizer()} functions a named numeric vector of estimated parameters and for \texttt{sampler()} functions parameter samples of class "mcmc" or "mcmc.list" (see package \texttt{coda}, Plummer et al. 2006). More details on the naming convention and the structure of the return value of \texttt{bamlss.frame()} are given in Section 4.1.

To ease the modeling process, all the single modeling steps presented in the above can be executed using the \texttt{bamlss} wrapper function \texttt{bamlss()}. The main arguments of \texttt{bamlss()} are
bamlss(formula, family = "gaussian", data = NULL,
transform = NULL, ## Pre-processing
optimizer = NULL, sampler = NULL, ## Estimation
samplestats = NULL, results = NULL, ...) ## Post-processing

where the first line basically represents the standard model frame specifications (see Chambers and Hastie 1992). All other arguments represent functions presented in Table 2 and can be exchanged. Note that the default for argument optimizer is the backfitting estimation function bfit() and the default for argument sampler is the GMCMC() sampling function.

The returned fitted model object is a list of class "bamlss", which is supported by several standard methods and extractor functions, such as plot(), summary() and predict().

As already exemplified in Section 2, using the model fitting wrapper function bamlss() it is straightforward to use different modeling approaches by simply exchanging the estimation engines. This feature can be particularly important in complex modeling situation, where good mixing of the MCMC algorithm requires very good starting values. One use case is presented in Section 5, where for stability reasons posterior mode estimates are obtained using the gradient boosting optimizer function boost(). Afterwards the MCMC sampling engine GMCMC() is applied with the boosting estimates as starting values.

4.1. The BAMLSS model frame

Similar to the well-known model.frame() function that is used, e.g., by the linear model fitting function lm(), or for generalized linear models glm(), the bamlss.frame() function extracts a “model frame” for fitting distributional regression models. Internally, the function parses model formulae, one for each parameter of the distribution, using the Formula package infrastructures (Zeileis and Croissant 2010) in combination with model.matrix() processing for linear effects and smooth.construct() processing of the mgcv package to setup design and penalty matrices for unspecified smooth function estimation (Wood 2019, see also, e.g., the documentation of function s() and te()).

The most important arguments are

bamlss.frame(formula, data = NULL, family = "gaussian",
weights = NULL, subset = NULL, offset = NULL,
na.action = na.omit, contrasts = NULL, ...)

The argument formula can be a classical model formulae, e.g., as used by the lm() function, or an extended bamlss formula including smooth term specifications like s() or te(), that is internally parsed by function bamlss.formula(). Note that the bamlss package uses special family objects, that can be passed either as a character without the "_bamlss" extension of the bamlss family name (see the manual ?bamlss.family for a list of available families), or the family function itself. In addition, all families of the gamlss (Stasinopoulos and Rigby 2019a) and gamlss.dist (Stasinopoulos and Rigby 2019b) package are supported.

The returned object, a named list of class "bamlss.frame", can be employed with the model fitting engines listed in Table 2. The most important elements used for estimation are:

- x: A named list, the elements correspond to the parameters that are specified within the family object. For each distribution parameter, the list contains all design and penalty matrices needed for modeling (see the upcoming example).
To better understand the structure of the "bamlss.frame" object a print method is provided. For illustration, we simulate data

R> set.seed(111)
R> d <- GAMart()

and set up a "bamlss.frame" object for a Gaussian distributional regression model including smooth terms. First, a model formula is needed

R> f <- list(
+   num ~ x1 + s(x2) + s(x3) + te(lon,lat),
+   sigma ~ x1 + s(x2) + s(x3) + te(lon,lat)
+ )

Afterwards the model frame can be computed with

R> bf <- bamlss.frame(f, data = d, family = "gaussian")

To keep the overview, there is also an implemented print method for "bamlss.frame" objects.

R> print(bf)

'bamlss.frame' structure:
$.call
$.model.frame
$.formula
$.family
$.terms
$.x
....$.mu
.....$.formula
.....$.fake.formula
.....$.terms
.....$.model.matrix
.....$.smooth.construct
....$.sigma
....$.formula
.....$.fake.formula
.....$.terms
.....$.model.matrix
.....$.smooth.construct
..$.y
...$.num
For writing a new estimation engine, the user can directly work with the \texttt{model.matrix} elements, for linear effects, and the \texttt{smooth.construct} list, for smooth effects respectively. The \texttt{smooth.construct} is a named list which is compiled using the \texttt{smoothCon()} function of the \texttt{mgcv} package using the generic \texttt{smooth.construct()} method for setting up smooth terms.

\begin{verbatim}
R> print(names(bf$x$mu$smooth.construct))
\end{verbatim}

\begin{verbatim}
[1] "s(x2)"    "s(x3)"    "te(lon,lat)"
\end{verbatim}

In this example, the list contains three smooth term objects for parameter \texttt{mu} and \texttt{sigma}.

As shown in Appendix C the \texttt{bamlss.frame()} function can also process special model terms, i.e., model terms that are not necessarily represented by a linear matrix vector product.

### 4.2. Family objects

Family objects are important building blocks in the design of BAMLSS models. They specify the distribution by collecting functions of the density, respective log-likelihood, first-order derivatives of the log-likelihood w.r.t. predictors (the score function), and (optionally) second-order derivatives of the log-likelihood w.r.t. predictors or their expectation (the Hessian).

The \texttt{bamlss} package can be easily extended by constructing families for specific tasks, i.e., problems for which a likelihood can be formulated. However, commonly used distributions are already implemented in \texttt{bamlss}; and the ones from the \texttt{gamlss} package can also be accessed through the \texttt{bamlss} package.

We illustrate how to build a \texttt{bamlss} family by hand along the Gaussian distribution, with density

$$f(y | \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma}} \cdot \exp \left(\frac{-(y - \mu)^2}{2\sigma^2}\right),$$

and log-likelihood function

$$\ell(\mu, \sigma | y) = -\frac{1}{2} \log(2\pi) - \log(\sigma) - \frac{(y - \mu)^2}{2\sigma^2},$$

for an individual observation. The sum of the log-likelihood function over all observations is the target function of the optimization problem.

In the distributional regression framework the parameters are linked to predictors by link functions,

$$\mu = \eta_\mu, \quad \log(\sigma) = \eta_\sigma.$$ 

For the Gaussian \(\mu\) and \(\sigma\) are linked to \(\eta_\mu\) and \(\eta_\sigma\) by the identity function and the logarithm, respectively.

The score functions in \texttt{bamlss} are the first derivatives of the log-likelihood w.r.t. the predictors:

$$s_\mu = \frac{\partial \ell}{\partial \eta_\mu} = \frac{\partial \ell}{\partial \mu} \cdot \frac{\partial \mu}{\partial \eta_\mu} = \frac{y - \mu}{\sigma^2},$$

and

$$s_\sigma = \frac{\partial \ell}{\partial \eta_\sigma} = \frac{\partial \ell}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial \eta_\sigma} = -1 + \frac{(y - \mu)^2}{\sigma^2}.$$
Table 3: Elements of the Gaussian distribution "bamlss.family" object.

For the second derivative of the log-likelihood we are able to obtain the negative expectation,
\[ E(-\partial^2 \ell / \partial \eta^2_\mu) = \sigma^{-2}, \]
and
\[ E(-\partial^2 \ell / \partial \eta^2_\sigma) = 2. \]

Now we have to write a function that returns a `family.bamlss` object (S3) which encapsulates functions for density, score and Hessian, and the names of the family, parameter and link functions. The required elements are listed in Table 3.

Merely all functions take as first argument the response `y` and as second argument a named list holding the evaluated parameters `par` of the distribution. The example implementation is shown in Appendix B.

Optionally, the "family.bamlss" object can be extended by functions for

- the cumulative distribution function `p(y, par, ...)`,
- the quantile function (the inverse cdf) `q(p, par)`,
- a random number generator `r(n, par)`,
- the log-likelihood `loglik(y, par)`,
- the expectation `mu(par, ...)`,
- initial values for optimization, which has to be a list containing a function for each parameter,
- ...

which can help to speed up optimization, or be convenient for predictions and simulations.

For a list of all implemented families, please see the documentation of `?bamlss.family`.

4.3. Estimation engines

Estimation engines in `bamlss` are usually based on the model frame setup function `bamlss.frame()` (see Section 4.1), i.e., the functions all have a `x` argument, which contains
all the necessary model and penalty matrices, and a \( y \) argument, which is the response (univariate or multivariate). In addition, an estimation engine usually has a family argument, which specifies the model to be estimated. However, this is not a mandatory argument, i.e., one could write an estimation function that is designed for one specific problem, only.

The modeling setup is best explained by looking at the main estimation engines provided by \texttt{bamlss}. The default optimizer using the \texttt{bamlss()} wrapper function is \texttt{bfit()}, which is a backfitting routine. The most important arguments are

\[
\texttt{bfit(x, y, family, start = NULL, weights = NULL, offset = NULL, \ldots)}
\]

The default sampling engine in \texttt{bamlss} is \texttt{GMCMC()}, again the most important arguments are

\[
\texttt{GMCMC(x, y, family, start = NULL, weights = NULL, offset = NULL, \ldots)}
\]

So basically, the arguments of the optimizer and the sampling function are the same, the main difference is the return value. In \texttt{bamlss} optimizer functions usually return a vector of estimated regression coefficients (parameters), while sampling functions return a matrix of parameter samples of class "mcmc" or "mcmc.list" (for details see the documentation of the \texttt{coda} package).

Internally, what the optimizer or sampling function is actually processing is not important for the \texttt{bamlss()} wrapper function as long as a vector or matrix of parameters is returned. For optimizer functions the return value needs to be named list with an element "parameters", the vector (also a matrix, e.g., for \texttt{lasso()} and \texttt{boost()} optimizers) of estimated parameters. The most important requirement to make use of all extractor functions like \texttt{summary.bamlss()}, \texttt{predict.bamlss()}, \texttt{plot.bamlss()}, \texttt{residuals.bamlss()}, etc., is to follow the naming convention of the returned estimates. The parameter names are based on the names of the distribution parameters as specified in the family object. For example, the family object \texttt{gaussian.bamlss()} has parameter names "mu" and "sigma"

\begin{verbatim}
R> gaussian_bamlss()$names
[1] "mu"    "sigma"
\end{verbatim}

Then, each distributional parameter can be modeled by parametric (linear) and nonlinear smooth effect terms. The parametric part is indicated with "p" and the smooth part with "s". The names of the parametric coefficients are the names of the corresponding model matrices as returned from \texttt{bamlss.frame()}. E.g., if two linear effects, with variables "x1" and "x2", enter the model for distributional parameter "mu", then the final names are "mu.p.x1" and "mu.p.x2". Similarly for the smooth parts, if we model a variable "x3" using a regression spline as provided by the \texttt{s()} function of the \texttt{mgcv} package, the name is based on the names that are used by \texttt{bamlss.frame()} for the \texttt{smooth.construct()} object. In this case the parameter names start with "mu.s.s(x3)". If this smooth term has 10 regression coefficients, then the final name must be

\begin{verbatim}
R> paste0("mu.s.s(x3)", ".b", 1:10)
[1] "mu.s.s(x3).b1" "mu.s.s(x3).b2" "mu.s.s(x3).b3"
[4] "mu.s.s(x3).b4" "mu.s.s(x3).b5" "mu.s.s(x3).b6"
\end{verbatim}
An example of how to setup an estimation engine for bamls for linear regression models is given in Appendix D. The example also provides details on the naming convention and return values of optimizer and sampler functions.

5. Flexible count regression for lightning reanalysis

This section illustrates the workflow with bamls along a small case study. We want to build a statistical model linking positive counts of cloud-to-ground lightning discharges to atmospheric quantities from a reanalysis dataset.

The region we focus on are the European Eastern Alps. Cloud-to-ground lightning discharges—detected by the Austrian Lightning Detection and Information System (ALDIS, Schulz, Cummins, Diendorfer, and Dorninger 2005)—are counted on grids with a mesh size of 32 km. The lightning observations are available for the period 2010–2018. The reanalysis data comes from the fifth generation of the ECMWF (European Centre for Medium-Range Weather Forecasts) atmospheric reanalyses of the global climate (Copernicus Climate Change Service 2017). ERA5 provides a globally complete and consistent pseudo-observations of the atmosphere using the laws of physics. The horizontal resolution is approx. 32 km, while the temporal resolution is hourly and covers the years from 1979 to present. In this example application we work only with a small subset of the data, which can be assessed from the accompanying R package FlashAustria (Simon 2019). The data is loaded with

```r
R> data("FlashAustria", package = "FlashAustria")
R> head(FlashAustriaTrain)
counts   d2m q_prof_PC1 cswc_prof_PC4 t_prof_PC1 v_prof_PC2
1 291.3184 -0.011472293 7.168725e-06 15.922548 2.5646172
2 283.5004  0.001007288 1.612870e-05 -9.758380 0.7955608
3 291.0506 -0.005590341 -3.226052e-06 20.274007 7.5535312
4 288.0358 -0.006293043 3.715074e-05 14.258116 5.8523424
5 288.4433 -0.005590341 7.168725e-06 20.274007 7.5535312
6 286.6035 -0.001597900 -3.195042e-06 -3.433136 -3.4291366
```

```r
R> nrow(FlashAustriaTrain)
[1] 12000
```
The motivation for this application is as follows: Lightning counts are not modeled within the atmospheric reanalyses. Lightning observations are only available for the period 2010–2018. With a statistical model on hand one could predict lightning counts for the time before 2010 and thus analyze lightning events in the past for which no observations are available.

The response of our statistical model are positive counts, with a mean of 13.61, and a variance of 1180.63. Thus, we are facing a truncated count data distribution which is highly overdispersive. In order to capture the truncation of the data and its overdispersion we employ a zero-truncated negative binomial distribution (Cameron and Trivedi 2013), which is specified by two parameters $\mu > 0$ and $\theta > 0$. $\mu$ is the expectation of the underlying untruncated negative binomial, and $\theta$ modifies the variance of the untruncated negative binomial by $\text{VAR}(\tilde{Y}) = \mu + \mu^2/\theta$, where $\tilde{Y}$ is a latent random variable following the underlying untruncated negative binomial distribution.

The zero-truncated negative binomial distribution is implemented as `ztnbinom_bamlss()` within `bamlss`. In order to specify smooth terms form both distributional parameter, the formula has to be a `list`. The first element specifies terms for the response `counts`, which is named $\mu$ in the `bamlss` family object. The second element specifies the formula for parameter $\theta$. Hence well known for their sampling properties, we are applying P-splines (Eilers and Marx 1996) for all terms. Specifying smooth terms within `bamlss` formulae builds on the `mgcv` infrastructure (Wood 2019) provided by `s()`, which leads to the following specification of the model (formula):

```r
R> f <- list(  
+   counts ~ s(d2m, bs = "ps") + s(q_prof_PC1, bs = "ps") +  
+   s(cswc_prof_PC4, bs = "ps") + s(t_prof_PC1, bs = "ps") +  
+   s(v_prof_PC2, bs = "ps") + s(sqrt_cape, bs = "ps"),  
+   theta ~ s(sqrt_lsp, bs = "ps")  
+ )
```

Now we have all ingredients on hand to feed the standard interface for statistical models in R: A formula `f`, a family `ztnbinom_bamlss()`, and a data set `FlashAustriaTrain`. Within the `bamlss()` call we also provide arguments which are passed forward to the optimizer and the sampler. We choose the gradient boosting optimizer `boost()` in order to find initial values for the default sampler `GMCMC()`. Gradient boosting proved to offer a very stable method for finding regression coefficients that serve as initial values for a MCMC sampler (Simon, Mayr, Umlauf, and Zeileis 2019). We set the number of iteration to 1000. For the sampling we allow another 1000 iterations as burn-in phase, and apply a thinning of the resulting chain of 5. Running `n.iter = 6000` iterations in total leads to 1000 MCMC samples in the end:

```r
R> set.seed(111)  
R> b <- bamlss(f, family = "ztnbinom", data = FlashAustriaTrain,  
+   optimizer = boost, maxit = 1000, ## Boosting arguments.  
+   thin = 5, burnin = 1000, n.iter = 6000) ## Sampler arguments.
```

logLik -36930.0 eps 0.0003 iteration 1000 qsel 7  
elapsed time: 5.31min  
Starting the sampler...  
|***************| 100%  0.00sec 27.76min
The model was fitted on a single core Intel i7-7700 CPU with 3.60GHz and 16 GB memory, on which the boosting took about 5.3 minutes and the MCMC sampling took about 27.8 minutes. As a first diagnostic we check the log-likelihood contributions of the individual terms during the boosting optimization (Figure 7).

R> pathplot(b, which = "loglik.contrib", intercept = FALSE)

After 1000 iterations the term \(s(q_{\text{prof\_PC1}}).\mu\) has the highest contribution to the log-likelihood with 344 followed by \(s(\sqrt{\text{cape}}).\mu\) with 212. The term of the parameter \(\theta\) \(s(\sqrt{\text{lsp}}).\theta\) has a relatively small contribution with 4. The overall message of this diagnostic is that the contributions to the log-likelihood at the end of the boosting procedure are very small and that the algorithm approached a stable state, which suggest that we retrieve reasonable initial values for the MCMC sampling.

The MCMC chains are investigated by looking directly at the traces of the chains and with the auto-correlation function of the chains.

R> plot(b, model = "mu", term = "s(\sqrt{\text{cape}})", which = "samples")

Figure 8 shows the traces and the auto-correlation functions for two regression coefficients of the term \(s(\sqrt{\text{cape}})\). The traces reveal samples around stables means. This suggests that the 1000 boosting iterations and the 1000 burn-in samples were sufficient in order to approach reasonable starting values for the sampling. The auto-correlation functions reveal that after the thinning hardly any correlation remains between consecutive samples.

As these diagnostics suggest that a reasonable initial state for the sampling has been found and the samples are independent draws from the posterior, one can go further and investigate the estimated effects. The boosting summary (Figure 7) revealed that the terms \(s(\sqrt{\text{cape}})\) and \(s(q_{\text{prof\_PC1}})\) had a large contribution for improving the fit. Looking at these effects...
Figure 8: MCMC trace (left panels) and auto-correlation (right panels) for two splines from the term $s(\sqrt{\text{cape}})$ of the model $\mu$.

illustrate how the atmospheric parameters of the reanalyses are related to lightning events (Figure 9), and thus help to understand the physics associated with lightning events. The effects are presented on the scale of the linear predictor, i.e., the log scale.

\begin{verbatim}
R> plot(b, term = c("s(sqrt_cape)", "s(q_prof_PC1)", "s(sqrt_lsp)"))
\end{verbatim}

$s(\sqrt{\text{cape}})$ reveals a monotonic increasing shape. In the range from 0–30 the effect increases linearly with small credible intervals. For higher values the effect flattens and shows large credible intervals which are associated with the small amount of data in that range. Physically the shape of the effect is meaningful as more convective available potential energy has the potential to lead to heavier lightning events. $s(q_{\text{prof\_PC1}})$ reveals areas of large credible intervals at the left and right bounds of the range due to small amount of data. In the mid-range an increasing effect is identified. As $q_{\text{prof\_PC1}}$ is the leading principal component of the vertical profile of specific humidity, one has to consider the corresponding spatial mode (not shown) for interpretation: Higher values of $q_{\text{prof\_PC1}}$ are linked to more moisture in the lower atmosphere, which is also available as a source of latent energy, i.e., energy that becomes free when water transfers from the gas to the liquid phase.

Finally it is interesting to look at the effect acting on the link scale of the parameter $\theta$, $s(\sqrt{\text{lsp}})$ (right panel in Figure 9). $\sqrt{\text{lsp}}$ is the square root of large scale precipitation, i.e., precipitation that is not linked to convective processes and thus it is not related to strong
lightning events. The effect shows following relationship: Higher values of \( \text{sqrt}_lsp \) lead to smaller \( \theta \), which increases the variance of the distribution.

Before applying the model, i.e., predicting lightning cases before 2010, we check the marginal calibration of the distribution by hanging rootogram, a tool popular for the evaluation of count data regression models (Kleiber and Zeileis 2016). First we predict the distributional parameter on out-of-sample data \text{FlashAustriaEval} for which lightning observations are on hand.

```r
R> fit <- predict(b, newdata = FlashAustriaEval, type = "parameter")
R> str(fit)

List of 2
$ mu : num [1:6000] 0.0159 0.0328 0.0126 0.0265 0.0458 ... 
$ theta: num [1:6000] 0.000706 0.000707 0.000712 0.000709 0.000704 ...
```

`predict()` returns a list, of which each element is named as a distributional parameter and contains by default a vector of predictions. Each prediction is the average of the predictions obtained by all MCMC samples. The resulting list can be used to derive further quantities by employing the functions of the \text{bamlss} family that can be extracted using `family()`.

```r
R> fam <- family(b)
R> fam

Family: ztnbinom
Link function: mu = log, theta = log
```
Derivative functions:
.. $ score
.. .. $ mu
.. .. $ theta
.. $ hess
.. .. $ mu
.. .. $ theta

The family contains functions to map the predictors to the parameter scale, density, cumulative distribution function, log-likelihood, and scores and Hessian. We apply the density to compute the expected frequencies of the positive counts. The function ..$d() takes the quantile as first argument, and the list with the parameters, as returned by predict(), as a second argument. The expected frequencies can then be computed by

\[ R> expect <- \text{sapply}(1:50, \text{function}(j) \text{sum}(\text{fam}$d(j, fit))) \]

In order to plot the rootogram, we have to name the vector and coerce it to an object of class table. The verifying observed frequencies can be directly obtained by table.

\[ R> \text{names(expect) <- 1:50} \]
\[ R> \text{expect <- as.table(expect)} \]
\[ R> \text{obsrvd <- table(FlashAustriaEval$counts)[1:50]} \]

The observed and expected frequencies can be plugged into the default method of rootogram from the countreg package (Zeileis, Kleiber, and Jackman 2008).

\[ R> \text{library("countreg")} \]
\[ R> \text{rootogram(obsrvd, expect, xlab = "}# Lightning Counts\", main = "Rootogram")} \]

The rootogram reveals reasonable calibration of the model though it is slightly underestimating the number of events with a single lightning discharge. Now given good convergence and sample characteristics of the gradient boosting optimizer and MCMC sampler, physically interpretable effects, and good out-of-sample calibration, we can take our model and predict a case for the period before 2010, for which no lightning data are available. The case of interest is a front moving from the West to the East on the Northern side of the Alps on 2001-09-15 and 2001-09-16. The case data FlashAustriaCase contains additional columns containing time and space information, and is of class sf (Pebesma 2018). We predict the parameters for this case, and derive the probability of observing 10 or more flashes within a grid box conditioned on a thunderstorm activity, by applying the cumulative distribution function ..$p of the family

\[ R> \text{library("sf")} \]
\[ R> \text{fit <- predict(b, newdata = FlashAustriaCase, type = "parameter")} \]
\[ R> \text{FlashAustriaCase$P10 <- 1 - fam$p(9, fit)} \]

We visualize this case by employing ggplot() (Wickham 2016), and the Oslo color scale from the colorspace package (Zeileis, Fisher, Hornik, Ihaka, McWhite, Murrell, Stauffer, and Wilke 2019). The country borders world are retrieved from the rnaturaleza package (South 2017).
Figure 10: Hanging rootogram for evaluating calibration of count data model on out-of-sample data. Red line indicates the expected frequencies on the square root scale. Gray bars indicate observed frequencies on square root scale hanging from the red line.

Figure 11: A probabilistic reconstruction of lightning counts occurred on September 15 2001 at 6 UTC, 17 UTC and 23 UTC and on September 16 2001 at 13 UTC, i.e., the probability of having observed 10 or more counts within one grid box.
\begin{verbatim}
R> library("ggplot2")
R> world <- rnaturalearth::ne_countries(scale = "medium", returnclass = "sf")
R> ggplot() + geom_sf(aes(fill = P10), data = FlashAustriaCase) +
  + scale_fill_continuous_sequential("Oslo", rev = TRUE) +
  + geom_sf(data = world, col = "white", fill = NA) +
  + coord_sf(xlim = c(7.95, 17), ylim = c(45.45, 50), expand = FALSE) +
  + facet_wrap(~time) + theme_minimal()
\end{verbatim}

The maps are shown in Figure 11 and reveal that the probability for strong lightning events
increases during 2001-09-15 between 6 and 17 UTC. During night time the front occurs, which
can be nicely seen at 23 UTC. The propagation of the front is blocked by the main Alpine
ridge located at 47° N. On the subsequent day 2001-09-16 one can see that the probability
on the downwind side of the Alps has increased.

Acknowledgments

Thorsten Simon acknowledges the funding by the Austrian Science Fund (FWF, grant no. P31836)

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A. Custom CRPS() function

The R package `scoringRules` (Jordan et al. 2019) provides tools for model calibration checks. A commonly used measure is the CRPS. Since the number of candidate distributions in BAMLSS is quite large, it can happen that the CRPS for some distributions is not implemented. In such a case the reader can implement the CRPS using numerical integration. The following R code implements the `CRPS()` to be used with `bamlss` and a numeric response, e.g., which can be used with the motorcycle accident model presented in Section 2.3.

```r
R> CRPS <- function(object, newdata = NULL) {
+   yname <- response_name(object)
+   fam <- family(object)
+   if(is.null(fam$p))
+     stop("no p() function in family object!")
+   if(is.null(newdata))
+     newdata <- model.frame(object)
+   n <- nrow(newdata)
+   crps <- rep(0, n)
+   par <- as.data.frame(predict(object, newdata = newdata, type = "parameter"))
+   for(i in 1:n) {
+     foo <- function(y) {
+       (fam$p(y, par[i, , drop = FALSE]) - 1 * (y >= newdata[[yname]][i]))^2
+     }
+     crps[i] <- integrate(foo, -Inf, Inf)$value
+   }
+   return(crps)
+ }
```

B. Gaussian family object

The following R code shows an example implementation of the Gaussian distribution as presented in Section 4.2.

```r
R> Gauss_bamlss <- function(...) {
+   f <- list(
+     "family" = "mygauss",
+     "names" = c("mu", "sigma"),
+     "links" = c(mu = "identity", sigma = "log"),
+     "d" = function(y, par, log = FALSE) {
+       dnorm(y, mean = par$mu, sd = par$sigma, log = log)
+     },
+     "p" = function(y, par, ...) {
+       pnorm(y, mean = par$mu, sd = par$sigma, ...)  
+     },
+     "r" = function(n, par) {
+       rnorm(n, mean = par$mu, sd = par$sigma)
+     }
+   )
+   return(f)
+ }
```
C. Special model terms

The default estimation engines \texttt{bfit()} and \texttt{GMCMC()} (also the gradient boosting optimizer function \texttt{boost()} in \texttt{bamlss}) provide support for the implementation of special model terms, i.e., model terms that cannot be represented by the \texttt{mgcv} smooth term constructor infrastructure. One simple example of such a special model term is a nonlinear growth curve, e.g., a nonlinear Gompertz curve

\[ f(x; \beta) = \beta_1 \cdot \exp(-\beta_2 \cdot \exp(-\beta_3 \cdot x)), \]

but also the lasso model term constructor \texttt{la()} presented in Section 2.2 is a special \texttt{bamlss} model term. The special model term constructor is needed in this case, since the growth curve is nonlinear in the parameters \( \beta \), hence, the default backfitting and sampling strategies cannot be applied. Fortunately, estimation algorithms in distributional regression can be split into separate updating equations (see also Section 3.2). This means that each model term can have its own updating function. The user interested in this feature only needs to write a new \texttt{smooth.construct()} and \texttt{Predict.matrix()} method.

The following \texttt{R} code implements a Gompertz growth model term which can be used by the default optimizer function \texttt{bfit()} and sampling function \texttt{GMCMC()} of the \texttt{bamlss} package. The new \texttt{smooth.construct()} method is
In principle, the setup is very similar to the smooth constructor functions provided by the mgcv package. Only few elements need to be added:

- **fit.fun()**: A function of the data $X$ and parameter vector $b$ that evaluates the fitted values.
- **update()**: An updating function to be used with optimizer bfit().
- **propose()**: A MCMC propose function to be used with sampler GMCMC().
- **prior()**: Function of the parameters $b$ that evaluates the log-prior. Note, additional functions can be grad() and hess that evaluate the first and second derivative of the log-prior w.r.t. the parameters $b$.
- **fixed**: Is the number of degrees of freedom fixed or not?
Figure 12: Estimated nonlinear effects on parameter $\mu$ and $\sigma$ of the simulated growth curve example. Gray shaded areas represent 95% credible intervals.

- **state**: This is a named list with starting values for the "parameters", the "fitted.values" and degrees of freedom "edf". Note that regression coefficients are always named with "b*" and shrinkage or smoothing variances with "tau2*" in the "parameters" vector.

- **special.npar**: How many parameters does this model term have in total? This is needed for internal setup, because the Gompertz function has three parameters but the design matrix only one column.

To compute predictions of this model term a new method for the `Predict.matrix()` function needs to be implemented, too.

```r
R> Predict.matrix.gc.smooth <- function(object, data, knots)
+ { 
+   X <- matrix(as.numeric(data[[object$term]]), ncol = 1)
+   X
+ }
```

Special model terms can then be used with the constructor function `s2()`. To illustrate the this feature in `bamlss`, we simulate heteroskedastic growth data with

$$y \sim N(\mu = 2 + 1/\left(1 + \exp(0.5 \cdot (15 - \text{time})\right)), \log(\sigma) = -3 + 2 \cdot \cos(\text{time}/30 \cdot 6 - 3))$$

and subsequently estimate the model with slice sampling (Neal 2003) for $\beta$ in the MCMC algorithm using the following R code

```r
R> set.seed(111)
R> d <- data.frame("time" = 1:30)
R> d$y <- 2 + 1 / (1 + exp(0.5 * (15 - d$time))) +
+   rnorm(30, sd = exp(-3 + 2 * cos(d$time/30 * 6 - 3)))
R> f <- list(
```
+ y ~ s2(time, bs = "gc"),
+ sigma ~ s(time)
+ )
R> b <- bamlss(f, data = d, optimizer = bfit, sampler = GMCMC)
R> plot(b)

The estimated effects are shown in Figure 12. The growth curve mean function estimate seems to fit the data quite well. Also, the nonlinear relationship for parameter $\sigma$ could be captured by the model.

In summary, in order to build up special bamlss model terms only a few things have to be considered. The example R code for the Gompertz smooth constructor given here is a good starting point for readers interested in using this feature.

D. Model fitting engines for linear regression

In the following, to explain the setup and the naming convention of estimation engines in more detail, we implement

- a new family object for simple linear models $y = x^T \beta + \varepsilon$ with $\varepsilon \sim N(0, \sigma^2)$,
- and set up an optimizer function,
- and additionally a MCMC sampling function.

For illustration, the family object is kept very simple, we only model the mean function in terms of covariates.

R> lm_bamlss <- function(...) {
+ f <- list(
+ "family" = "LM",
+ "names" = "mu",
+ "links" = "identity",
+ "d" = function(y, par, log = FALSE) {
+ sigma <- sqrt(sum((y - par$mu)^2) / (length(y) - .lm_bamlss.p))
+ dnorm(y, mean = par$mu, sd = sigma, log = log)
+ },
+ "p" = function(y, par, ...) {
+ sigma <- sqrt(sum((y - par$mu)^2) / (length(y) - .lm_bamlss.p))
+ pnorm(y, mean = par$mu, sd = sigma, ...)
+ }
+ }
+ class(f) <- "family.bamlss"
+ return(f)
+ }

Now, for setting up the estimation functions we first simulate some data using the GAMart() function, afterwards the necessary "bamlss.frame" can be created with
R> d <- GAMart()
R> bf <- bamlss.frame(num ~ x1 + x2, data = d, family = "lm")
R> print(bf)

'bamlss.frame' structure:

..$ call
..$ model.frame
..$ formula
..$ family
..$ terms
..$ x
  ...$ mu
    ...$ formula
    ...$ fake.formula
    ...$ terms
    ...$ model.matrix
    ..$ y
    ...$ num

As noted above, the object is a named list with elements "x" and "y", which will be passed to the estimation functions. For the moment, since we only implement a linear model, we need to work with the linear model matrix that is part of the bf object.

R> head(bf$x$mu$model.matrix)

   (Intercept)   x1   x2
1   1.0 .2905102 .3265972
2   1.0 .5090036 .0304738
3   1.0 .3900498 .8245305
4   1.0 .3650458 .2485895
5   1.0 .5219909 .1908983
6   1.0 .1977914 .6598312

and the response y

R> head(bf$y)

     num
1 0.2232725
2 0.2479576
3 0.1221580
4 -0.1370822
5 -0.1108988
6 -0.1011208

to setup the optimizer function with:
R> lm.opt <- function(x, y, ...) 
+ { 
+   ## Only univariate response.
+   y <- y[[1L]]
+   
+   ## For illustration this is easier to read.
+   X <- x$mu$model.matrix
+   
+   ## Estimate model parameters.
+   par <- drop(chol2inv(chol(crossprod(X))) %*% crossprod(X, y))
+   
+   ## Set parameter names.
+   names(par) <- paste0("mu.p.", colnames(X))
+   
+   ## Return estimated parameters and fitted values.
+   rval <- list(
+     "parameters" = par,
+     "fitted.values" = drop(X %*% par),
+     "edf" = length(par),
+     "sigma" = drop(sqrt(crossprod(y - X %*% par) / (length(y) - ncol(X))))
+   )
+   
+   ## Set edf within .GlobalEnv for the
+   ## loglik() function in the lm_bamlss() family.
+   .lm_bamlss.p <<- length(par)
+   
+   return(rval)
+ }

This optimizer function can already be used with the bamlss() wrapper function and all extractor functions are readily available.

R> f <- num ~ x1 + poly(x2, 5) + poly(x3, 5)
R> b <- bamlss(f, data = d, family = "lm", optimizer = lm.opt, sampler = FALSE)
R> summary(b)

Call:
bamlss(formula = f, family = "lm", data = d, optimizer = lm.opt, sampler = FALSE)
---
Family: LM
Link function: mu = identity
---
Formula mu:
---
num ~ x1 + poly(x2, 5) + poly(x3, 5)
Parametric coefficients:

\[
\begin{align*}
\text{(Intercept)} & \quad 0.199 \\
x1 & \quad -0.653 \\
poly(x2, 5)1 & \quad -1.791 \\
poly(x2, 5)2 & \quad 2.014 \\
poly(x2, 5)3 & \quad 0.474 \\
poly(x2, 5)4 & \quad -1.752 \\
poly(x2, 5)5 & \quad 0.743 \\
poly(x3, 5)1 & \quad -0.303 \\
poly(x3, 5)2 & \quad 4.273 \\
poly(x3, 5)3 & \quad 0.050 \\
poly(x3, 5)4 & \quad 0.572 \\
poly(x3, 5)5 & \quad 0.144 \\
\end{align*}
\]

---

Optimizer summary:

- \( \text{edf} = 12 \) \( \text{sigma} = 0.2257 \)

---

\[
R> nd <- \text{data.frame("x2" = seq(0, 1, length = 100))}
R> nd$p <- \text{predict(b, newdata = nd, term = "x2")}
\]

Plot the estimated effect of variable \( x2 \).

\[
R> \text{plot2d(p ~ x2, data = nd)}
\]

The next step is to setup a full Bayesian MCMC sampling function. Fortunately, if we assume multivariate normal priors for the regression coefficients and an inverse Gamma prior for the variance, a Gibbs sampler with multivariate normal and inverse Gamma full conditionals can be created. The MCMC algorithm consecutively samples for \( t = 1, \ldots, T \) from the full conditionals
\[
\beta^{(t)} | \cdot \sim N \left( \mu^{(t-1)}_{\beta}, \Sigma^{(t-1)}_{\beta} \right)
\]
and
\[
\sigma^{2(t)} | \cdot \sim IG \left( a^{(t-1)}, b^{(t-1)} \right),
\]
where \( IG(\cdot) \) is the inverse Gamma distribution for sampling the variance parameter. The covariance matrix for \( \beta \) is given by
\[
\Sigma_{\beta} = \left( \frac{1}{\sigma^2} X^\top X + \frac{1}{\sigma^2} M^{-1} \right)^{-1}
\]
and the mean
\[
\mu_{\beta} = \Sigma_{\beta} \left( \frac{1}{\sigma^2} X^\top y + \frac{1}{\sigma^2} M^{-1} m \right),
\]
where \( m \) is the prior mean and \( M \) the prior covariance matrix. Similarly, for \( \sigma^2 \) parameters \( a' \) and \( b' \) are computed by
\[
a' = a + \frac{n}{2} + \frac{p}{2}
\]

and

\[ b' = b + \frac{1}{2} (y - X\beta)^\top (y - X\beta) + \frac{1}{2} (\beta - \mathbf{m})^\top M^{-1} (\beta - \mathbf{m}), \]

where \( a \) and \( b \) are usually set small, e.g., with \( a = 1 \) and \( b = 0.0001 \), such that the prior is flat and uninformative.

We can implement the MCMC algorithm in the following sampling function

```r
R> lm.mcmc <- function(x, y, start = NULL,
+ n.iter = 12000, burnin = 2000, thin = 10,
+ m = 0, M = 1e+05,
+ a = 1, b = 1e-05,
+ verbose = TRUE, 
+ ...)  
+ {  
+ ## How many samples are saved?  
+ itrthin <- seq.int(burnin, n.iter, by = thin)  
+ nsaves <- length(itrthin)  
+  
+ ## Only univariate response.  
+ y <- y[[1L]]  
+  
+ ## For illustration this is easier to read.  
+ X <- x$mu$model.matrix  
+  
+ ## Again, set edf within .GlobalEnv for the  
+ ## loglik() function in the lm_bamlss() family.  
+ .lm_bamlss.p <<- ncol(X)  
+  
+ ## Number of observations and parameters.  
+ n <- length(y)  
+ p <- ncol(X)  
+  
+ ## Matrix saving the samples.  
+ samples <- matrix(0, nsaves, p + 1L)  
+  
+ ## Stick to the naming convention.  
+ pn <- paste0("mu.p.", colnames(X))  
+ colnames(samples) <- c(  
+  pn,       ## Regression coefficients and  
+ "sigma"   ## variance samples.  
+  )  
+  
+ ## Setup coefficient vector,  
+ ## again, use correct names.  
+ beta <- rep(0, p)  
+ names(beta) <- pn  
+ sigma <- sd(y)  
+ ...}
```
## Check for starting values obtained, e.g., from lm.optim() from above.

```r
if(!is.null(start)) {
  sn <- names(start)
  for(j in names(beta)) {
    if(j %in% sn)
      beta[j] <- start[j]
  }
}
```

## Process prior information.

```r
m <- rep(m, length.out = p)
M <- rep(M, length.out = p)
if(!is.matrix(M))
  M <- diag(M)
Mi <- solve(M)
```

## Precompute cross products.

```r
XX <- crossprod(X)
Xy <- crossprod(X, y)
```

## Inverse gamma parameter.

```r
a <- a + n / 2 + p / 2
```

## Start sampling.

```r
ii <- 1
for(i in 1:n.iter) {
  ## Sampling sigma
  b2 <- b + 1 / 2 * t(y - X %*% beta) %*% (y - X %*% beta) + 
  1 / 2 * t(beta - m) %*% Mi %*% (beta - m)
  sigma2 <- sqrt(1 / rgamma(1, a, b2))
  
  ## Sampling beta.
  sigma2 <- 1 / sigma2
  Sigma <- chol2inv(chol(sigma2i * XX + sigma2i * Mi))
  mu <- Sigma %*% (sigma2i * Xy + sigma2i * Mi %*% m)
  beta <- MASS::mvrnorm(1, mu, Sigma)
  
  if(i %in% itrthin) {
    samples[ii, pn] <- beta
    samples[ii, "sigma"] <- sqrt(sigma2)
    ii <- ii + 1
  }
  if(verbose) {
    if(i %% 1000 == 0)
      cat("iteration:", i, "\n")
  }
}
The new sampling function can be directly used with the `bamlss()` wrapper

```r
R> b <- bamlss(f, data = d, family = "lm", optimizer = lm.opt, sampler = lm.mcmc)
```

```r
iteration: 1000
iteration: 2000
iteration: 3000
iteration: 4000
iteration: 5000
iteration: 6000
iteration: 7000
iteration: 8000
iteration: 9000
iteration: 10000
iteration: 11000
iteration: 12000
```

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

Call:  
`bamlss(formula = f, family = "lm", data = d, optimizer = lm.opt,`  
`  sampler = lm.mcmc)`

---

Family: LM  
Link function: mu = identity

*---*  
Formula mu:  
---

`num ~ x1 + poly(x2, 5) + poly(x3, 5)`

---

Parametric coefficients:  

|            | Mean  | 2.5%  | 50%  | 97.5% | parameters |
|------------|-------|-------|------|-------|------------|
| (Intercept)| 0.19937 | 0.11443 | 0.19799 | 0.28402 | 0.199 |
| x1         | -0.65380 | -0.79612 | -0.65227 | -0.51375 | -0.653 |
| poly(x2, 5)1 | -1.79249 | -2.71924 | -1.79813 | -0.86320 | -1.791 |
| poly(x2, 5)2 | 2.00010 | 1.08057 | 1.99022 | 2.88333 | 2.014 |
| poly(x2, 5)3 | 0.48731 | -0.48780 | 0.49488 | 1.49446 | 0.474 |
| poly(x2, 5)4 | -1.78055 | -2.66888 | -1.78927 | -0.81921 | -1.752 |
poly(x2, 5)5 0.73783 -0.28079 0.74257 1.72215 0.743
poly(x3, 5)1 -0.29363 -1.25928 -0.29305 0.56080 -0.303
poly(x3, 5)2 4.29066 3.36496 4.28125 5.26903 4.273
poly(x3, 5)3 0.03256 -0.98550 0.05819 1.01670 0.050
poly(x3, 5)4 0.57143 -0.36514 0.58563 1.48913 0.572
poly(x3, 5)5 0.13204 -0.81059 0.13434 1.07470 0.144
---
Sampler summary:

DIC = 23.3951 pd = 52.4174 runtime = 2.483
---
Optimizer summary:

edf = 12 sigma = 0.2257
---

R> ## Predict for all terms including 95% credible intervals
R> nd$x1 <- nd$x3 <- seq(0, 1, length = 100)
R> for(j in c("x1", "x2", "x3")) {
+   nd[[paste0("p.", j)]] <- predict(b, newdata = nd, term = j,
+     FUN = c95, intercept = FALSE)
+ }

The estimated effects can be plotted with:

R> par(mfrow = c(1, 3))
R> plot2d(p.x1 ~ x1, data = nd, fill.select = c(0, 1, 0, 1), lty = c(2, 1, 2))
R> plot2d(p.x2 ~ x2, data = nd, fill.select = c(0, 1, 0, 1), lty = c(2, 1, 2))
R> plot2d(p.x3 ~ x3, data = nd, fill.select = c(0, 1, 0, 1), lty = c(2, 1, 2))

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