gamboostLSS: boosting generalized additive models for location, scale and shape

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useR! 2011
Motivation: Munich rental guide

Aim:
- Provide precise point predictions and prediction intervals for the net-rent of flats in the city of Munich.

Data:
- Covariates: 325 (mostly) categorical, 2 continuous and 1 spatial
- Observations: 3016 flats

Problem:
- Heteroscedasticity found in the data

Idea
Model not only the expected mean but also the variance ⇒ GAMLSS
The GAMLSS model class

Generalized Additive Models for Location, Scale and Shape

\[ g_1(\mu) = \eta_\mu = \beta_0\mu + \sum_{j=1}^{p_1} f_{j\mu}(x_j) \]  
"location"

\[ g_2(\sigma) = \eta_\sigma = \beta_0\sigma + \sum_{j=1}^{p_2} f_{j\sigma}(x_j) \]  
"scale"

\[ \vdots \]

- Introduced by Rigby and Stasinopoulos (2005)
- Flexible alternative to generalized additive models (GAM)
- Up to four distribution parameters are regressed on the covariates.
- Every distribution parameter is modeled by its own predictor and an associated link function \( g_k(\cdot) \).
Current fitting algorithm

The `gamlss` package

Fitting algorithms for a large amount of distribution families are provided by the R package `gamlss` (Stasinopoulous and Rigby, 2007).

- Estimation is based on a penalized likelihood approach.
- Modified versions of back-fitting (as for conventional GAMs) are used.

These algorithms work remarkably well in many applications, but:

- It is not feasible for high-dimensional data ($p \gg n$).
- No spatial effects are implemented.
- Variable selection is based on generalized AIC, which is known to be unstable.
  - “More work needs to be done here” (Stasinopoulous and Rigby, 2007).
Optimization problem for GAMLSS

- The task is to model the distribution parameters of the conditional density \( f_{\text{dens}}(y|\mu, \sigma, \nu, \tau) \)

- The optimization problem can be formulated as

\[
\begin{aligned}
(\hat{\mu}, \hat{\sigma}, \hat{\nu}, \hat{\tau}) &\leftarrow \arg\min_{\theta} \mathbb{E}_{Y,X} \left[ \rho \left( Y, \eta_{\mu}(X), \eta_{\sigma}(X), \eta_{\nu}(X), \eta_{\tau}(X) \right) \right] \\
\end{aligned}
\]

with loss function \( \rho = -l \), i.e., the negative log-likelihood of the response distribution:

\[
l = \sum_{i=1}^{n} \log \left[ f_{\text{dens}}(y_i|\theta_i) \right] = \sum_{i=1}^{n} \log \left[ f_{\text{dens}}(y_i|\mu_i, \sigma_i, \nu_i, \tau_i) \right]
\]

- Maximum likelihood approach
Alternative to ML: Component-wise boosting

Boosting

- minimizes empirical risk (e.g., negative log likelihood)
- in an iterative fashion
- via functional gradient descent (FGD).

In boosting iteration $m + 1$

- Compute (negative) gradient of the loss function and plug in the current estimate
  \[
  u_i^{[m+1]} = - \frac{\partial \rho(y_i, \eta)}{\partial \eta} \bigg|_{\eta=\hat{\eta}_i^{[m]}}
  \]

- Estimate $u_i^{[m+1]}$ via base-learners (i.e., simple regression models)
- Update: use only the best-fitting base-learner; add a small fraction $\nu$ of this estimated base-learner (e.g., 10%) to the model

▶ Variable selection intrinsically within the fitting process
Boosting for GAMLSS models

- Boosting was recently extended to risk functions with multiple components (Schmid et al., 2010)
- **Idea** ▶ Use partial derivatives instead of gradient
- Specify a set of base-learners — one base-learner per covariate
- Fit each of the base-learners **separately** to the partial derivatives
- **Cycle** through the partial derivatives within each boosting step
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\[
\frac{\partial \rho}{\partial \eta_\mu}(y_i, \hat{\mu}^{[m]}, \hat{\sigma}^{[m]}, \hat{\nu}^{[m]}, \hat{\tau}^{[m]}) \quad \text{update} \quad \hat{\eta}_\mu^{[m+1]} \Rightarrow \hat{\mu}^{[m+1]},
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\[
\frac{\partial \rho}{\partial \eta_\mu} (y_i, \hat{\mu}_m, \hat{\sigma}_m, \hat{\nu}_m, \hat{\tau}_m) \quad \xrightarrow{\text{update}} \quad \text{best fitting BL} \quad \hat{\eta}_\mu^{m+1} \rightarrow \hat{\mu}_{m+1},
\]

\[
\frac{\partial \rho}{\partial \eta_\sigma} (y_i, \hat{\mu}_m^{m+1}, \hat{\sigma}_m, \hat{\nu}_m, \hat{\tau}_m) \quad \xrightarrow{\text{update}} \quad \text{best fitting BL} \quad \hat{\eta}_\sigma^{m+1} \rightarrow \hat{\sigma}_{m+1},
\]

\[
\frac{\partial \rho}{\partial \eta_\nu} (y_i, \hat{\mu}_m^{m+1}, \hat{\sigma}_m^{m+1}, \hat{\nu}_m, \hat{\tau}_m) \quad \xrightarrow{\text{update}} \quad \text{best fitting BL} \quad \hat{\eta}_\nu^{m+1} \rightarrow \hat{\nu}_{m+1},
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\]

\[
\frac{\partial \rho}{\partial \eta_\tau}(y_i, \hat{\mu}^{[m+1]}, \hat{\sigma}^{[m+1]}, \hat{\nu}^{[m+1]}, \hat{\tau}^m) \quad \text{update} \quad \hat{\eta}_\tau^{[m+1]} \Rightarrow \hat{\tau}^{[m+1]}.
\]
Variable selection and shrinkage

- The main tuning parameter are the stopping iterations $m_{\text{stop},k}$. They control variable selection and the amount of shrinkage.
  - If boosting is stopped before convergence only the most important variables are included in the final model.
  - Variables that have never been selected in the updated step, are excluded.
  - Due to the small increments added in the update step, boosting incorporates shrinkage of effect sizes (compare to LASSO), leading to more stable predictions.
- For large $m_{\text{stop},k}$ boosting converges to the same solution as the original algorithm (in low-dimensional settings).
- The selection of $m_{\text{stop},k}$ is normally based on resampling methods, optimizing the predictive risk.
Data example: Munich rental guide

To deal with heteroscedasticity, we chose a three-parametric t-distribution with

$$\mathbb{E}(y) = \mu \quad \text{and} \quad \text{Var}(y) = \sigma^2 \frac{\text{df}}{\text{df} - 2}$$

For each of the parameters $\mu$, $\sigma$, and $\text{df}$, we consider the candidate predictors

$$
\eta_{\mu_i} = \beta_0 \mu + x_i^T \beta_{\mu} + f_{1,\mu}(\text{size}_i) + f_{2,\mu}(\text{year}_i) + f_{\text{spat},\mu}(s_i), \\
\eta_{\sigma_i} = \beta_0 \sigma + x_i^T \beta_{\sigma} + f_{1,\sigma}(\text{size}_i) + f_{2,\sigma}(\text{year}_i) + f_{\text{spat},\sigma}(s_i), \\
\eta_{\text{df}_i} = \beta_0 \text{df} + x_i^T \beta_{\text{df}} + f_{1,\text{df}}(\text{size}_i) + f_{2,\text{df}}(\text{year}_i) + f_{\text{spat},\text{df}}(s_i).
$$

Base-learners

- Categorical variables: Simple linear models
- Continuous variables: P-splines
- Spatial variable: Gaussian MRF (Markov random fields)
Package `gamboostLSS`

- Boosting for GAMLSS models is implemented in the R package `gamboostLSS` (now available on CRAN).
- Package relies on the well tested and mature boosting package `mboost`.
- Lots of the `mboost` infrastructure is available in `gamboostLSS` as well (e.g., base-learners & convenience functions).
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**Now let’s start and have a short look at some code!**
## Install package mboost: (we use the R-Forge version as the bmrf base-learner is not yet included in the CRAN version)

```r
install.packages("mboost",
+ repos = "http://r-forge.r-project.org")
```

## Install and load package gamboostLSS:

```r
install.packages("gamboostLSS")
library("gamboostLSS")
```
(Simplified) code to fit the model

> ## Load data first, and load boundary file for spatial effects
> ## Now set up formula:
> form <- paste(names(data)[1], " ~ ",
>     paste(names(data)[-c(1, 327, 328, 329)], collapse = " + "),
>     " + bbs(wfl) + bbs(bamet) + bmrf(region, bnd = bound)"
> form <- as.formula(form)
> form

nmqms ~ erstbezg + dienstwg + gebmeist + gebgruen + hzkohojn +
    ... +
    bbs(wfl) + bbs(bamet) + bmrf(region, bnd = bound)

> ## Fit the model with (initially) 100 boosting steps
> mod <- gamboostLSS(formula = form, families = StudentTLSS(),
>                     control = boost_control(mstop = 100,
>                     trace = TRUE),
>                     baselearner = bols,
>                     data = data)

[ 1] .................................................. -- risk: 3294.323
[ 41] .................................................. -- risk: 3091.206
[ 81] ..................
Final risk: 3038.919
(Simplified) code to fit the model (ctd.)

```r
> ## optimal number of boosting iterations fund by 3-dimensional
> ## cross-validation on a logarithmic grid resulted in
> ## 750 (mu), 108 (sigma), 235 (df) steps;
> ## Let model run until these values:
> mod[c(750, 108, 235)]
>
> ## Let’s look at the number of variables per parameter:
> sel <- selected(mod)
> lapply(sel, function(x) length(unique(x)))

$mu
[1] 115

$sigma
[1] 31

$df
[1] 7

> ## (Very) sparse model (only 115, 31 and 5 base-learners out of 328)
```
(Simplified) code to fit the model (ctd.)

```r
> ## Now we can look at the estimated parameters
> ## e.g., the effect of roof terrace on the mean
> coef(mod, which = "dterasn", parameter = "mu")

$'bols(dterasn)'
   (Intercept)  dterasn
-0.004254606  0.293792997

> ## We can also easily plot the estimated smooth effects:
> plot(mod, which = "bbs(wfl)", parameter = "mu",
+      xlab = "flat size (in square meters)", type = "l")
```

![Graph showing the estimated smooth effects of flat size on the mean with a curve that decreases to 0 and then increases again.](graph.png)
Estimated spatial effects obtained for the high-dimensional GAMLSS for distribution parameters $\mu$ and $\sigma$. For the third parameter $\text{df}$, the corresponding variable was not selected.
Results: prediction intervals

95% prediction intervals based on the quantiles of the modeled conditional distribution. Coverage probability GAMLSS 93.93% (92.07-95.80); coverage probability GAM 92.23% (89.45-94.32).
Summary

- As gamboostLSS relies on mboost, we have a well tested, mature back end.
- The base-learners offer great flexibility when it comes to the type of effects (linear, non-linear, spatial, random, monotonic, . . .).
- Boosting is feasible even if \( p \gg n \).
- Variable selection is included in the fitting process. Additional shrinkage leads to more stable results.

The algorithm is implemented in the R add-on package gamboostLSS now available on CRAN.
Further literature


