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

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useR! 2011

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MEDIZINISCHE FAKULTÄT

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 $\Rightarrow$ **GAMLSS**

The GAMLSS model class

Generalized Additive Models for Location, Scale and Shape

$$g_1(\mu) = \eta_\mu = \beta_{0\mu} + \sum_{j=1}^{p_1} f_{j\mu}(x_j) \qquad \text{“location”}$$

$$g_2(\sigma) = \eta_\sigma = \beta_{0\sigma} + \sum_{j=1}^{p_2} f_{j\sigma}(x_j) \qquad \text{“scale”}$$

$$\vdots$$

- 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` (Stasinopoulus 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"* (Stasinopoulus 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

$$\underbrace{(\hat{\mu}, \hat{\sigma}, \hat{\nu}, \hat{\tau})}_{\boldsymbol{\theta}} \longleftarrow \underset{\eta_\mu, \eta_\sigma, \eta_\nu, \eta_\tau}{\operatorname{argmin}} \mathbb{E}_{Y,X}\Big[\rho\big(Y, \underbrace{\eta_\mu(X), \eta_\sigma(X), \eta_\nu(X), \eta_\tau(X)}_{\boldsymbol{\eta}}\big)\Big]$$

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

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

  - 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
$$u_i^{[m+1]} = - \left. \frac{\partial \rho(y_i, \eta)}{\partial \eta} \right|_{\eta = \hat{\eta}_i^{[m]}}$$
- 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 ν 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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$$\frac{\partial \rho}{\partial \eta_{\boldsymbol{\mu}}}(y_i, \hat{\mu}^{[m]}, \hat{\sigma}^{[m]}, \hat{\nu}^{[m]}, \hat{\tau}^{[m]}) \quad \xrightarrow[\text{best fitting BL}]{\text{update}} \quad \hat{\eta}_{\mu}^{[\mathbf{m+1}]} \Longrightarrow \hat{\mu}^{[\mathbf{m+1}]} \ ,$$

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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

$$\mathbb{E}(y) = \mu \qquad \text{and} \qquad \mathbb{V}\mathsf{ar}(y) = \sigma^2 \frac{\mathsf{df}}{\mathsf{df} - 2}$$

For each of the parameters μ, σ, and df, we consider the **candidate** predictors

$$\begin{aligned}
\eta_{\mu_i} &= \beta_{0\mu} + x_i^\top \beta_\mu + f_{1,\mu}(\mathsf{size}_i) + f_{2,\mu}(\mathsf{year}_i) + f_{\mathsf{spat},\mu}(s_i) \ , \\
\eta_{\sigma_i} &= \beta_{0\sigma} + x_i^\top \beta_\sigma + f_{1,\sigma}(\mathsf{size}_i) + f_{2,\sigma}(\mathsf{year}_i) + f_{\mathsf{spat},\sigma}(s_i) \ , \\
\eta_{\mathsf{df}_i} &= \beta_{0\mathsf{df}} + x_i^\top \beta_{\mathsf{df}} + f_{1,\mathsf{df}}(\mathsf{size}_i) + f_{2,\mathsf{df}}(\mathsf{year}_i) + f_{\mathsf{spat},\mathsf{df}}(s_i) \ .
\end{aligned}$$

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!

Package gamboostLSS

```
> ## Install package mboost: (we use the R-Forge version as the
> ## bmrf base-learner is not yet included in the CRAN version)
> install.packages("mboost",
+                  repos = "http://r-forge.r-project.org")
> ## Install and load package gamboostLSS:
> install.packages("gamboostLSS")
> library("gamboostLSS")
```

(Simplified) code to fit the model

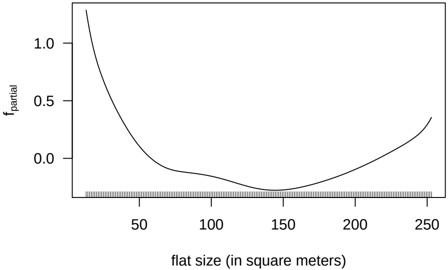
```
> ## Load data first, and load boundary file for spatial effects
> ## Now set up formula:
> form <- paste(names(data)[1], " ~ ",
                paste(names(data)[-c(1, 327, 328, 329)], collapse = " + "),
                " + bbs(wfl) + bbs(bamet) + bmrf(region, bnd = bound)")
> form <- as.formula(form)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

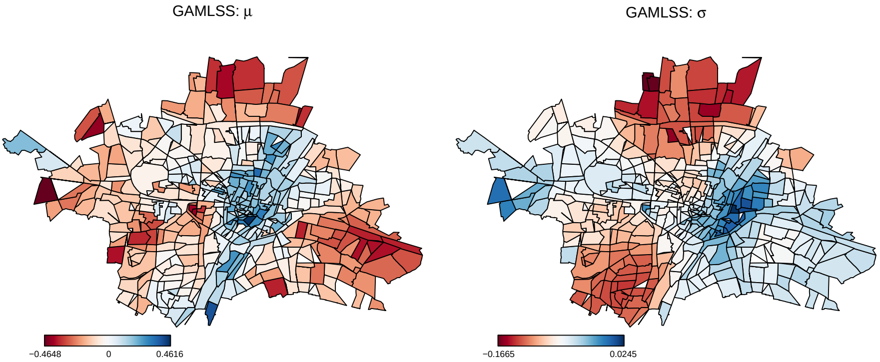
```
> ## optimal number of boosting iterations fund by 3-dimensional
> ## cross-validation on a logarithmic grid resulted in
> ## 750 (mu), 108 (sigma), 235 (df) steps;
> ## Let model run until these values:
> mod[c(750, 108, 235)]
>
> ## Let's look at the number of variables per parameter:
> sel <-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

```
> ## 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")
```

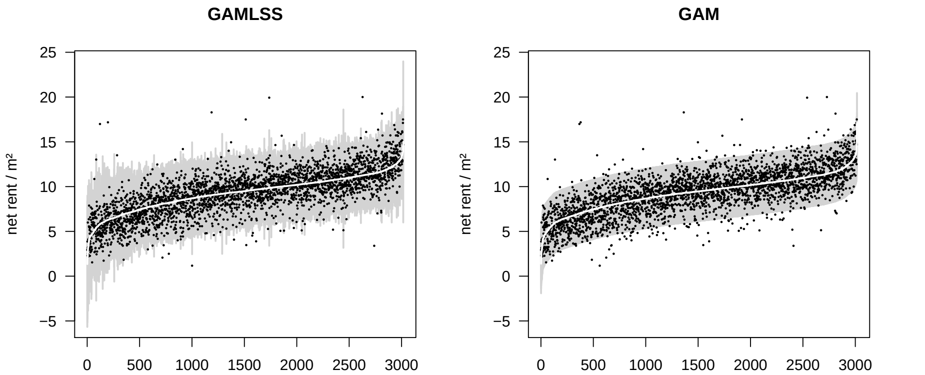


Results: spatial effects



Estimated spatial effects obtained for the high-dimensional GAMLSS for distribution parameters μ and σ. For the third parameter `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

- ▷ Mayr, A., N. Fenske, B. Hofner, T. Kneib and M. Schmid, (2010). GAMLSS for high-dimensional data – a flexible approach based on boosting. *Journal of the Royal Statistical Society, Series C (Applied Statistics)*, accepted.
- ▷ B. Hofner, A. Mayr, N. Fenske, and M. Schmid, (2010). gamboostLSS: Boosting Methods for GAMLSS Models. R package version 1.0-1.

- Bühlmann, P. and Hothorn, T., (2007). Boosting algorithms: Regularization, prediction and model fitting. *Statistical Science*, **22**, 477-522.
- Rigby, R. A. and Stasinopoulos, D. M., (2005). Generalized additive models for location, scale and shape. *Applied Statistics*, **54**, 507-554.
- Schmid, M., S. Potapov, A. Pfahlberg and T. Hothorn, (2010). Estimation and regularization techniques for regression models with multidimensional prediction functions . *Statistics and Computing*, **20**, 139-150.