Gradient boosting in Markov-switching generalized additive models for location, scale and shape

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Abstract

We propose a novel class of flexible latent-state time series regression models which we call Markov-switching generalized additive models for location, scale and shape. In contrast to conventional Markov-switching regression models, the presented methodology allows us to model different state-dependent parameters of the response distribution — not only the mean, but also variance, skewness and kurtosis parameters — as potentially smooth functions of a given set of explanatory variables. In addition, the set of possible distributions that can be specified for the response is not limited to the exponential family but additionally includes, for instance, a variety of Box-Cox-transformed, zero-inflated and mixture distributions. We propose an estimation approach based on the EM algorithm, where we use the gradient boosting framework to prevent overfitting while simultaneously performing variable selection. The feasibility of the suggested approach is assessed in simulation experiments and illustrated in a real-data setting, where we model the conditional distribution of the daily average price of energy in Spain over time.

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1 Introduction

In recent years, latent-state models — particularly hidden Markov models (HMMs) — have become increasingly popular tools for time series analyses. In many applications, the data at hand follow some pattern within some periods of time but reveal different stochastic properties during other periods (Zucchini et al., 2016). Typical examples are economic time series, e.g. share returns, oil prices or bond yields, where the functional relationship between response and explanatory variables may differ in periods of high and low economic growth, inflation or unemployment (Hamilton, 1989). Since their introduction by Goldfeld and Quandt (1973) nearly half a century ago, Markov-switching regression models, i.e. time series regression models where the functional relationship between response and explanatory variables is subject to state-switching controlled by an unobservable Markov chain, have emerged as the method of choice to account for the dynamic patterns described above.

While Markov-switching regression models are typically restricted to modeling the mean of the response (treating the remaining parameters as nuisance and constant across observations), it often appears that other parameters — including variance, skewness and kurtosis parameters — may depend on explanatory variables as well rather than being constant (Rigby and Stasinopoulos, 2005). A motivating example to have in mind is the daily average price of energy, which we present in detail in Section 5 for Spain as specific case study. When the energy market is in a calm state, which implies relatively low prices alongside a moderate volatility, then the oil price exhibits positive correlation with the mean of the conditional energy price distribution, but the variance is usually constant across observations. In contrast, when the energy market is nervous, which implies relatively high and volatile prices, then also the variance of energy prices is strongly affected by the oil price. This latter possible pattern cannot be addressed with existing
Markov-switching regression models. As a consequence, price forecasts may severely under- or overestimate the associated uncertainty, by neglecting the strong heteroscedasticity in the process. This is problematic in scenarios where interest lies not only in the expected prices, but also quantiles, e.g. when the costs of forecast errors are asymmetric.

Since their introduction in the seminal work of Rigby and Stasinopoulos (2005) a little more than a decade ago, generalized additive models for location, scale and shape (GAMLSS) have emerged as the standard framework for distributional regression models, where not only the mean, but also other parameters of the response distribution are modeled as potentially smooth functions of a given set of explanatory variables. Over the last decade, GAMLSS have been applied in a variety of fields, ranging from the analysis of insurance (Heller et al., 2007) and long-term rainfall data (Villarini et al., 2010) over phenological research (Hudson, 2010) and energy studies (Voudouris et al., 2011) to clinical applications, including long-term survival models (de Castro et al., 2010), childhood obesity (Beyerlein et al., 2008) and measurement errors (Mavr et al., 2017).

GAMLSS are applied primarily to data where it is reasonable to assume that the given observations are independent of each other. This is rarely the case when the data have a time series structure. In fact, when the data are collected over time, as e.g. daily energy prices, then the functional relationship between response and explanatory variables may actually change over time. This results in serially correlated residuals due to an under- or overestimation of the true functional relationship. To exploit the flexibility of GAMLSS also within time series settings, we propose a novel class of flexible latent-state time series regression models which we call Markov-switching GAMLSS (MS-GAMLSS). In contrast to conventional Markov-switching regression models, the presented methodology allows to model different state-dependent parameters of the response distribution as potentially smooth functions of a given set of explanatory variables.

A practical challenge that emerges with the flexibility of MS-GAMLSS is the potentially high dimension of the set of possible model specifications. Each of the parameters of the response distribution varies across two or more states, and each of the associated predictors may involve several explanatory variables, the effect of which may even need
Figure 1: In Section 2, we introduce the components of MS-GAMLSS and discuss the underlying dependence assumptions, which considers features from both HMMs and GAMLSS. In Section 3, we derive the MS-gamboostLSS algorithm, which incorporates gradient boosting into MS-GAMLSS.

to be estimated nonparametrically. Thus, a grid-search approach for model selection, e.g. based on information criteria, is usually practically infeasible. We therefore derive the MS-gamboostLSS algorithm for model fitting, which incorporates the gradient boosting framework into MS-GAMLSS. Gradient boosting emerged from the field of machine learning, but was later adapted to estimate statistical models (c.f. Mayr et al., 2014). The basic idea is to iteratively apply simple regression functions (which are denoted as base-learners) for each potential explanatory variable one-by-one and select in every iteration only the best performing one. The final solution is then an ensemble of the selected base-learner fits including only the most important variables. The design of the algorithm thus leads to automated variable selection and is even feasible for high-dimensional data settings, where the number of variables exceeds the number of observations.

The paper is structured as follows: In Section 2 we introduce the components of MS-GAMLSS and discuss the underlying dependence assumptions. In Section 3 we derive the MS-gamboostLSS algorithm and give a brief overview of related topics, including model selection. The synergy of HMMs and GAMLSS, which lies at the core of this work, is illustrated in Figure 1. In Section 4 we assess the suggested approach in simulation experiments, where we consider both linear and nonlinear base-learners. In Section 5 we illustrate the proposed methodology in a real-data setting, where we model the conditional distribution of the daily average price of energy in Spain over time.
2 Model formulation and dependence structure

In this section, we introduce the model formulation and dependence structure of MS-GAMLSS, which extends the closely related but less flexible and in fact nested class of Markov-switching generalized additive models (MS-GAMs, Langrock et al., 2017).

2.1 The state process

MS-GAMLSS comprise two stochastic processes, one of which is hidden and the other one is observed. The hidden process, \( \{S_t\}_{t=1,\ldots,T} \), which is referred to as the state process, is modeled by a discrete-time, \( N \)-state Markov chain. Assuming the Markov chain to be time-homogeneous, we summarize the state transition probabilities, i.e. the probabilities of switching from state \( i \) at time \( t \) to state \( j \) at time \( t + 1 \), in the \( N \times N \) transition probability matrix (t.p.m.) \( \Gamma \), with elements

\[
\gamma_{ij} = \Pr (S_{t+1} = j | S_t = i),
\]

\( i, j = 1, \ldots, N \). The initial state probabilities, i.e. the probabilities of the process being in the different states at time 1, are summarized in the row vector \( \delta \), with elements

\[
\delta_i = \Pr (S_1 = i),
\]

\( i = 1, \ldots, N \). If the Markov chain is assumed to be stationary, which is adequate in many applications, then the initial distribution is the stationary distribution, i.e. the solution to the equation system \( \delta \Gamma = \delta \) subject to \( \sum_{i=1}^{N} \delta_i = 1 \) (Zucchini et al., 2016). If the Markov chain is not assumed to be stationary, then the initial state probabilities are parameters which need to be estimated. The state process is completely specified by the initial state and the state transition probabilities.

Throughout this paper we consider first-order Markov chains, i.e. we assume that the state process satisfies the Markov property, \( \Pr(S_{t+1}|S_1, \ldots, S_t) = \Pr(S_{t+1}|S_t), t = \)
Figure 2: Dependence structure in Markov-switching generalized additive models for location, scale and shape.

1, . . . , T − 1. This simplifying dependence assumption is heavily exploited in the likelihood calculations provided in Section 3. While certainly being a strong assumption, in practice it is often a good proxy for the actual dependence structure, and could in fact be relaxed to higher-order Markov chains if deemed necessary (Zucchini et al., 2016).

2.2 The state-dependent process

The observed process, \{Y_t\}_{t=1,...,T}, which is referred to as the state-dependent process, can take either discrete or continuous values. We denote the conditional probability density function (p.d.f.) or, in the discrete case, probability mass function (p.m.f.), of \(Y_t\), by

\[
\begin{align*}
  f_Y (y_t; \theta_t^{(s_t)}) &= f_Y (y_t; \theta_1^{(s_t)}, \ldots, \theta_K^{(s_t)}).
\end{align*}
\]

(3)

Here \(\theta_t^{(s_t)} = (\theta_1^{(s_t)}, \ldots, \theta_K^{(s_t)})\) is the parameter vector associated with the distribution assumed for the response \(Y_t\). It depends both on the current state, \(s_t\), and on the explanatory variables at time \(t\), \(x_t = (x_{1t}, \ldots, x_{Pt})\), with \(P\) denoting the number of variables included in the model. The first parameter of the response distribution, \(\theta_1^{(s_t)}\), often denotes the conditional mean of \(Y_t\). Depending on the distributional family assumed, the other parameters may relate to the conditional variance, the conditional skewness and the conditional kurtosis, respectively, though other parameters are also possible. The set of possible distributions that can be specified for the response is not limited to the
The exponential family; in fact, any parametric distribution (including Box-Cox-transformed, zero-inflated and mixture distributions) can be considered. In principle, even more than four parameters could be considered, which however is of minor practical relevance and therefore omitted in the notation.

The variables $Y_1, \ldots, Y_T$ are assumed to be conditionally independent of each other given the states and the explanatory variables, as illustrated in the graphical model depicted in Figure 2. As the parameters are possibly constrained (the conditional variance, for instance, typically needs to be strictly positive), we introduce a monotonic link function $g_k(\theta_{kt}^{(s_t)})$ for each parameter $\theta_{kt}^{(s_t)}$, $k = 1, \ldots, 4$, which maps the latter onto some real-valued predictor function $\eta_k^{(s_t)}(x_t)$, the choice of which is determined by the respective parameter constraints. For instance, the log-link function, $g_k(\theta_{kt}^{(s_t)}) = \log(\eta_k^{(s_t)}(x_t))$, is typically chosen for the conditional variance, such that the inverse function, $\theta_{kt}^{(s_t)} = \exp(\eta_k^{(s_t)}(x_t))$, is strictly positive. The form of the predictor function is determined by the specification of the base-learners, the discussion of which is subject of Section 3.2.

3 Model fitting

In this section, we derive the MS-gamboostLSS algorithm to estimate the state transition probabilities (1), the initial state probabilities (2) and the state-dependent parameters of the response distribution in (3).

3.1 The MS-gamboostLSS algorithm

The MS-gamboostLSS algorithm comprises an outer and an inner cycle, which combine two different model fitting procedures in a joint algorithm: The outer cycle is the EM algorithm [Dempster et al., 1977; Baum et al., 1970; Welch, 2003], which is a popular method for iteratively maximizing the likelihood of a statistical model in the presence of missing data and has become one of the standard procedures for model fitting in HMMs. It is particularly useful in the context of MS-GAMLSS, as the hidden states can be regarded
as missing data. The inner cycle is a weighted version of the gamboostLSS algorithm (Mayr et al., 2012), which is exploited to carry out one part of the EM algorithm, namely the estimation of the state-dependent parameters of the response distribution in (3).

The missing data — more precisely, functions of the missing data — can be estimated, which is referred to as the expectation (E) step. Based on the obtained estimates, the complete-data log-likelihood (CDLL; i.e. the joint log-likelihood of the observations and and the states) is then maximized with respect to the state transition probabilities (1), the initial state probabilities (2) and the state-dependent parameters of the response distribution in (3), which is referred to as the maximization (M) step.

The complete-data log-likelihood: We represent the state sequence \( \{S_t\}_{t=1,...,T} \) (i.e., the missing data) by the binary random variables \( u_i(t) = 1_{S_t=i} \) and \( v_{ij}(t) = 1_{S_{t-1}=i, S_t=j} \) for \( i, j = 1, \ldots, N \) and \( t = 1, \ldots, T \) (i.e., functions of the missing data). Assuming the \( u_i(t) \)'s and \( v_{ij}(t) \)'s to be observed, the CDLL can be written as

\[
\text{CDLL} = \log \left( \delta_{s_1} \prod_{t=2}^{T} \gamma_{s_{t-1}s_t} \prod_{t=1}^{T} f_Y \left( y_t; \theta_t^{(s_t)} \right) \right) \\
= \log (\delta_{s_1}) + \sum_{t=2}^{T} \log (\gamma_{s_{t-1}s_t}) + \sum_{t=1}^{T} \log (f_Y \left( y_t; \theta_t^{(s_t)} \right)) \\
= \sum_{i=1}^{N} u_i(1) \log (\delta_i) + \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{t=2}^{T} v_{ij}(t) \log (\gamma_{ij}) + \sum_{i=1}^{N} \sum_{t=1}^{T} u_i(t) \log (f_Y \left( y_t; \theta_t^{(i)} \right)) .
\]

Note that the CDLL consists of three separate summands, each of which only depends on

i) \( \mathbf{\delta} = (\delta_i), i = 1, \ldots, N \), ii) \( \mathbf{\Gamma} = (\gamma_{ij}), i, j = 1, \ldots, N \), and iii) \( \mathbf{\theta}_t = (g_k^{-1}(\eta_k^{(i)}(x_t))), i = 1, \ldots, N, k = 1, \ldots, 4 \), which considerably simplifies the maximization in the M step. Since the \( u_i(t) \)'s and \( v_{ij}(t) \)'s are not observable, we first need to replace them by their conditional expectations, \( \hat{u}_i(t) \) and \( \hat{v}_{ij}(t) \), respectively.

In order to compute these conditional expectations, we require the forward and backward probabilities: The forward probabilities, \( \alpha_t(i) = f(y_1, \ldots, y_t, S_t = i|x_1, \ldots, x_t) \), are summarized in the row vectors \( \mathbf{\alpha}_t = (\alpha_t(1), \ldots, \alpha_t(N)) \), which are calculated via the
forward algorithm by applying the recursion

\[
\alpha_1 = \delta \mathbf{P}(y_1)
\]
\[
\alpha_t = \alpha_{t-1} \mathbf{P} (y_t),
\]
t = 2, \ldots, T, where \( \mathbf{P}(y_t) = \text{diag}(f_Y(y_t; \theta_t^{(1)}), \ldots, f_Y(y_t; \theta_t^{(N)})). \) The backward probabilities, \( \beta_t(j) = f(y_{t+1}, \ldots, y_T | S_t = j, \mathbf{x}_{t+1}, \ldots, \mathbf{x}_T), \) are summarized in the row vectors \( \beta_t = (\beta(1), \ldots, \beta(N)) \), which are evaluated via the backward algorithm by applying the recursion

\[
\beta_T = 1
\]
\[
\beta_t^\top = \mathbf{P} (y_{t+1}) \beta_{t+1}^\top,
\]
t = T - 1, \ldots, 1, with \( \mathbf{P}(y_{t+1}) \) as defined above. We let \( \alpha_t^{[m]}(i) \) and \( \beta_t^{[m]}(j) \) denote the forward and backward probabilities estimated in the \( m \)-th iteration, which are computed using the predictors obtained in the \( m - 1 \)-th iteration (or offset values in the case of the first iteration).

The \( m \)-th E step involves the computation of the conditional expectations of the \( u_i(t) \)'s and \( v_{ij}(t) \)'s given the current parameter estimates, which leads to the following results:

1. Since \( \hat{u}_i(t) = \Pr(S_t = i | y_1, \ldots, y_T, \mathbf{x}_1, \ldots, \mathbf{x}_T) = f(y_1, \ldots, y_t, S_t = i | \mathbf{x}_1, \ldots, \mathbf{x}_T) \)

   \[
   f(y_{t+1}, \ldots, y_T | S_t = i, \mathbf{x}_1, \ldots, \mathbf{x}_T) / f(y_1, \ldots, y_T | \mathbf{x}_1, \ldots, \mathbf{x}_T)
   \]

   and \( f(y_1, \ldots, y_T | \mathbf{x}_1, \ldots, \mathbf{x}_T) = \sum_{i=1}^{N} f(y_1, \ldots, y_T, S_t = i | \mathbf{x}_1, \ldots, \mathbf{x}_T), \) it follows immediately from the definition of the forward and backward probabilities that

   \[
   \hat{u}_i^{[m]}(t) = \frac{\alpha_t^{[m]}(i) \beta_t^{[m]}(i)}{\sum_{i=1}^{N} \alpha_T^{[m]}(i)},
   \]

   \( t = 1, \ldots, T, i = 1, \ldots, N. \)

2. Since \( \hat{v}_{ij}(t) = \Pr(S_{t-1} = i, S_t = j | y_1, \ldots, y_T, \mathbf{x}_1, \ldots, \mathbf{x}_T) = f(y_1, \ldots, y_{t-1}, S_{t-1} = i | \mathbf{x}_1, \ldots, \mathbf{x}_T) \Pr(S_t = j | S_{t-1} = i) f(y_t, \ldots, y_T | S_t = j, \mathbf{x}_1, \ldots, \mathbf{x}_T) / f(y_1, \ldots, y_T | \mathbf{x}_1, \ldots, \mathbf{x}_T) \),
\(x_T\), it follows immediately from the definition of the forward, backward and state transition probabilities that

\[
\hat{v}^{[m]}_{ij}(t) = \frac{\alpha_{i-1}^{[m]}(i) \hat{\gamma}^{[m-1]}_{ij} f_Y(y_t; \hat{\theta}_i^{(j)[m-1]}) \beta_{i}^{[m]}(j)}{\sum_{j=1}^{N} \alpha_{j}^{[m]}(j)}, \tag{7}
\]

\(t = 1, \ldots, T, i, j = 1, \ldots, N.\)

The \(m\)-th M step involves the maximization of the CDLL with the \(u_i(t)\)'s and \(v_{ij}(t)\)'s replaced by their current conditional expectations with respect to the model parameters:

1. As only the first term in the CDLL depends on \(\delta_i\), using a Lagrange multiplier to ensure \(\sum_{i=1}^{N} \hat{\delta}^{[m]}_{i} = 1\) results in

\[
\hat{\delta}^{[m]}_{i} = \frac{\hat{u}^{[m]}_{i}(1)}{\sum_{i=1}^{N} \hat{u}^{[m]}_{i}(1)} = \hat{u}^{[m]}_{i}(1), \tag{8}
\]

\(i = 1, \ldots, N.\)

2. As only the second term in the CDLL depends on \(\gamma_{ij}\), using a Lagrange multiplier to ensure \(\sum_{j=1}^{N} \hat{\gamma}^{[m]}_{ij} = 1, i = 1, \ldots, N,\) results in

\[
\hat{\gamma}^{[m]}_{ij} = \frac{\sum_{t=2}^{T} \hat{v}^{[m]}_{ij}(t)}{\sum_{j=1}^{N} \sum_{t=2}^{T} \hat{v}^{[m]}_{ij}(t)}, \tag{9}
\]

\(i, j = 1, \ldots, N.\)

3. As only the third term in the CDLL depends on the state-dependent parameters of the response distribution in (3), the optimization problem effectively reduces to maximizing the weighted log-likelihood of a separate, conventional GAMLSS for each state, where the \(t\)-th observation is weighted by \(\hat{u}^{[m]}_{i}(t)\). We can therefore exploit the gamboostLSS algorithm (Mayr et al., 2012) to iteratively maximize this weighted log-likelihood. In particular, we consider the computationally more efficient non-cyclical variant of the gamboostLSS algorithm (Thomas et al., 2017):
- Initialize the additive predictors \( \hat{\eta}^{(i)[0]}_k(x_t), i = 1, \ldots, N, k = 1, \ldots, 4, t = 1, \ldots T \) with offset values. For each additive predictor, specify a set of base-learners \( h^{(i)}_{k1}(x_{1t}), \ldots, h^{(i)}_{k4J_i}(x_{J_i t}) \) (e.g. simple linear models or penalized B-splines, i.e. P-splines; Eilers and Marx, 1996), where \( J_i^k \) denotes the cardinality of the set of base-learners specified for \( \eta^{(i)}_k(x_t) \).

- For \( i = 1 \) to \( N \):
  - For \( n = 1 \) to \( n^{(i)}_{\text{stop}} \):
    * For \( k = 1 \) to \( 4 \):
      - Compute the gradients of the CDLL with respect to \( \eta^{(i)}_k(x_t) \) (using the current estimates \( \hat{u}^{[m]}_i(t) \) and \( \hat{\theta}^{(i)[n-1]}_t = (g_k^{-1}(\eta^{(i)[n-1]}_k(x_t)), k = 1, \ldots, 4) \), \( t = 1, \ldots, T \), and fit each of the base-learners contained in the set of base-learners specified for \( \eta^{(i)}_k(x_t) \) to these gradients.
      - Select the best-fitting base-learner \( h^{(i)}_{kj*}(x_{j*t}) \) by the residual sum of squares of the base-learner fit with respect to the gradients,
      \[
      j^* = \arg\min_{j \in 1, \ldots, J_i^k} \sum_{t=1}^{T} (\nabla^{(i)}_{kt} - \hat{h}^{(i)}_{kj}(x_{jt}))^2.
      \]
      * Select, among the base-learners selected the previous loop, the best-fitting base-learner \( \hat{h}^{(i)}_{k^*j*}(x_{j*t}) \) by the weighted log-likelihood,
      \[
      k^* = \arg\max_{k \in 1, \ldots, 4} \sum_{t=1}^{T} \hat{u}^{[m]}_i(t) \log \left( f_Y \left( y_t; \hat{\theta}^{(i)[n-1]}_t \right) \right),
      \]
      where \( \hat{\theta}^{(i)[n-1]}_t \) is replaced by its potential update, \( g_k^{-1}(\eta^{(i)[n-1]}_k(x_t) + sl \).
\(\hat{h}_{k^*}(x_{j^*})\), to **update** the corresponding predictor,

\[
\eta_{k^*}[n](x_t) = \eta_{k^*}[n-1](x_t) + \text{sl} \cdot \hat{h}_{k^*}(x_{j^*})
\]

where \(0 < \text{sl} < 1\) is some small step length (typically, \(\text{sl} = 0.1\)).

- Set \(\eta_{k}[n](x_t) = \eta_{k}[n-1](x_t)\) for all \(k \neq k^*\).

- **Use** the predictors obtained in the final iteration as estimates obtained in the

  \(m\)th M step, \(\hat{\eta}_{k}[m](x_t) = \eta_{k}[\text{stop}](x_t)\) for all \(i, k\).

The MS-gamboostLSS algorithm alternates between the E and the M step, each of which involves \(\eta_{\text{stop}}\) boosting iterations for each state, \(i\), until some convergence threshold, e.g. based on the difference between the CDLLs obtained in two consecutive iterations, is satisfied.

### 3.2 Specification of base-learners

The specification of base-learners, \(h_{k^*}(x_{j^*})\), which are used to fit the gradient vectors, is crucial, as they define the type of predictor effect: If the base-learners have a linear form, then the resulting fit is also linear, whereas if nonlinear base-learners are chosen, then this fit may also be nonlinear. Generally, base-learners can be any kind of prediction functions — in the classical machine learning context gradient boosting is most often applied with trees or stumps as base-learners (Ridgeway, 1999). In the case of boosting algorithms for statistical modeling, it is, however, reasonable to select regression-type functions that can be combined to additive models (Mayr et al., 2014).

Due to their high flexibility, popular base-learners are P-splines (Eilers and Marx, 1996). They are typically applied with fixed low degrees of freedom (strong penalization) which are not tuned for the different boosting iterations. However, as the same P-spline base-learner can be selected as best-performing base-learner and updated in several boosting iterations, the resulting solution can have arbitrarily large complexity (i.e. wiggliness). The complexity increases as the number of boosting iterations increases. More
advanced base-learners are interaction terms (e.g. based on tensor product P-splines), random or spatial effects (e.g. based on Markov random fields). For an overview of available base-learners, see Mayr et al. (2012).

3.3 Choice of the number of boosting iterations

The stopping iterations, \( n_{\text{stop}}^{(i)} \), are the main tuning parameters for boosting algorithms. They control the variable selection properties of the algorithm and the smoothness of the estimated effects. They represent the classical trade-off between variance and bias in statistical modeling: Using more boosting iterations leads to larger and more complex models with smaller bias but larger variance, while stopping the algorithm earlier leads to sparser, less complex models with less variance but larger bias. Without early stopping, i.e. running the algorithm until convergence, the resulting fit converges to the maximum likelihood estimate (Mayr et al., 2012) (if this estimate exists for the given model).

Choosing an optimal number of boosting iterations is typically achieved via \( K \)-fold cross validation. For some set \( \Lambda = n_{\text{stop}}^{(1)} \times \cdots \times n_{\text{stop}}^{(N)} \subset \mathbb{N}^N \) we follow Celeux and Durand (2008) and proceed in the following way: First, we split the data into \( K \) distinct partitions (typically, \( K \geq 10 \)), estimate the model based on \( K - 1 \) partitions and compute the out-of-sample log-likelihood for the remaining partition (which is straightforward using the forward algorithm from Section 3.1). This procedure is repeated \( K \) times, i.e. until each partition has been out-of-sample once. The score of interest is the average out-of-sample log-likelihood over all partitions, where the number of boosting iterations corresponding to the highest score is chosen.

3.4 Selecting the number of states

The choice of the number of states, \( N \), is a rather difficult task — while the vast majority of Markov-switching regression models appearing in the literature assume two states without any critical reasoning, there actually exists a variety of different methods for order selection in HMMs, which basically fall in two categories: On the one hand, a cross-
validated likelihood approach can be used, as described in Section 3.3. On the other hand, information criteria such as Akaike’s Information Criterion, the Bayesian Information Criterion (Zucchini et al., 2016) or the Integrated Completed Likelihood Criterion (Celeux and Durand, 2008; Biernacki et al., 2013) can be considered, all of which result in a compromise between goodness of fit and model complexity.

One problem in practice, however, is that information criteria often tend to favor overly complex models. Real data typically exhibit more structure than can actually be captured by the model, which e.g. is the case if the true state-dependent distributions are too complex to be fully modeled by some (rather simple) parametric distribution or if certain temporal patterns are neglected in the model formulation. In the case of MS-GAMLSS, additional states may be able to capture this further structure. As a consequence, the goodness of fit increases, which may outweigh the higher model complexity. However, as models with too many states are usually difficult to interpret and are therefore often not desired, information criteria should be considered as a rough guidance rather than as a deterministic decision rule, which should be treated with some caution. For an in-depth discussion of pitfalls, practical challenges and pragmatic solutions regarding order selection in HMMs, see Pohle et al. (2017).

4 Simulation experiments

To assess the performance of the suggested approach, we present two different simulation settings, where we consider linear (Section 4.1) and nonlinear (Section 4.2) relationships between the explanatory variables and the parameters of the response distribution.

4.1 Linear setting

For the linear setting, we use simple linear models as base-learners. In each of 100 simulation runs, we simulated 500 realizations from a 2-state Markov chain, \( \{ S_t \}_{t=1,\ldots,500} \), with off-diagonal t.p.m. entries \( \gamma_{ij} = 0.05 \), \( i, j = 1, 2 \), \( i \neq j \), and initial state probabilities
\( \delta_i = 0.5, \ i = 1, 2 \). Based on the simulated state sequence, we then draw 500 observations from a negative binomial distribution with state-dependent p.m.f.

\[
f_Y \left( y_t; \theta_1^{(s_t)}, \theta_2^{(s_t)} \right) = \frac{\Gamma \left( y_t + \theta_2^{(s_t)} \right)}{\Gamma(y_t + 1) \Gamma \left( \theta_2^{(s_t)} \right)} \left( \frac{\theta_1^{(s_t)}}{\theta_2^{(s_t)} + 1} \right)^{y_t},
\]

where

\[
\log(\theta_1^{(1)}) = \eta_1^{(1)}(x_t) = 2 + 2x_{1t} + \sum_{j=2}^{100} 0x_{jt}
\]

\[
\log(\theta_1^{(2)}) = \eta_1^{(2)}(x_t) = 2 - 2x_{1t} + \sum_{j=2}^{100} 0x_{jt}
\]

\[
\log(\theta_2^{(1)}) = \eta_2^{(1)}(x_t) = 2x_{1t} + \sum_{j=2}^{100} 0x_{jt}
\]

\[
\log(\theta_2^{(2)}) = \eta_2^{(2)}(x_t) = -2x_{1t} + \sum_{j=2}^{100} 0x_{jt}
\]

and \( x_{jt} \sim \text{uniform}(-1, 1), \ j = 1, \ldots, 100, \ t = 1, \ldots, 500 \). To assess the variable selection performance, we included 99 noninformative explanatory variables in each predictor. The stopping iterations were chosen via 20-fold cross validation over the grid \( \Lambda = n_{\text{stop}}^{(1)} \times n_{\text{stop}}^{(2)} \), \( n_{\text{stop}}^{(1)} = n_{\text{stop}}^{(2)} = (100, 200, 400, 800) \), where the average chosen number of boosting iterations was 435 (state 1) and 468 (state 2).

The sample means of the estimated off-diagonal t.p.m. entries, \( \hat{\gamma}_{12} \) and \( \hat{\gamma}_{21} \), were obtained as 0.047 (standard deviation: 0.020) and 0.047 (0.019), respectively, which apparently is very close to the true values. The estimated state-dependent coefficients obtained in 100 simulation runs are displayed in Figures 3 and 4, respectively: For \( \theta_1^{(s_t)} \), the estimated coefficients are slightly shrunk towards zero, while for \( \theta_2^{(s_t)} \), the shrinkage effect is quite large. The informative covariates were — on average — selected in 98.5% of the cases (100.0% for \( \theta_1^{(s_t)} \) and 97.0% for \( \theta_2^{(s_t)} \)), while the noninformative ones were — on average — selected in 10.6% of the cases (13.4% for \( \theta_1^{(s_t)} \) and 7.7% for \( \theta_2^{(s_t)} \)), which
on the one hand indicates that the variable selection works quite well but on the other hand that there is a tendency towards too many covariates being included in the model (this apparently is a problem related to boosting in general rather than a specific one related to the MS-gamboostLSS algorithm, see e.g. the simulation experiments presented in Mayr et al., 2012).

Using a 3.6 GHz Intel® Core™ i7 CPU, the average computation time was 1.4 minutes for a (single) model (i.e. for a given number of boosting iterations), which is remarkably fast considering the fact that it involves variable selection among 100 potential explanatory variables.

### 4.2 Nonlinear setting

Encouraged by the performance in the linear setting, we next present a nonlinear setting using P-splines as base-learners, again simulating 500 realizations from a 2-state Markov chain with off-diagonal t.p.m. entries $\gamma_{ij} = 0.05$, $i, j = 1, 2$, $i \neq j$ and initial state prob-
abilities $\delta_i = 0.5$, $i, j = 1, 2$. We then draw 500 observations from a normal distribution with state-dependent p.d.f.

$$f_Y(y_t; \theta_{1t}^{(s_t)}, \theta_{2t}^{(s_t)}) = \frac{1}{\sqrt{2\pi \theta_{2t}^{(s_t)^2}}} \exp \left( -\frac{(y_t - \theta_{1t}^{(s_t)})^2}{2\theta_{2t}^{(s_t)^2}} \right),$$

where

$$\theta_{1t}^{(1)} = \eta_{1_t}^{(1)}(x_t) = 2 + 2 \sin(\pi (x_{1t} - 0.5)) + \sum_{j=2}^{100} 0x_{jt}$$

$$\theta_{1t}^{(2)} = \eta_{1_t}^{(2)}(x_t) = -2 - \sin(\pi (x_{1t} - 0.5)) + \sum_{j=2}^{100} 0x_{jt}$$

$$\log(\theta_{2t}^{(1)}) = \eta_{2_t}^{(1)}(x_t) = \sin(\pi (x_{1t} - 0.5)) + \sum_{j=2}^{100} 0x_{jt}$$

$$\log(\theta_{2t}^{(2)}) = \eta_{2_t}^{(2)}(x_t) = -2 \sin(\pi (x_{1t} - 0.5)) + \sum_{j=2}^{100} 0x_{jt}$$

and $x_{jt} \sim \text{uniform}(-1, 1)$, $j = 1, \ldots, 100$, $t = 1, \ldots, 500$. The stopping iterations were again chosen via 20-fold cross validation over the grid $\Lambda = n_{\text{stop}}^{(1)} \times n_{\text{stop}}^{(2)}$, $n_{\text{stop}}^{(1)} = n_{\text{stop}}^{(2)} = (25, 50, 100, 200)$, where the average chosen number of boosting iterations was 141.5 (state 1) and 177 (state 2).

The sample means of the estimated off-diagonal t.p.m. entries, $\hat{\gamma}_{12}$ and $\hat{\gamma}_{21}$, were obtained as 0.050 (0.014) and 0.051 (0.016), respectively. The estimated state-dependent effects obtained in 100 simulation runs are displayed in Figures 5 and 6, respectively: As in Section 4.1 we observe a shrinkage effect (especially for the larger effects, i.e. the effects of $x_{1t}$ on $\eta_{1_t}^{(1)}(x_t)$ and $\eta_{2_t}^{(2)}(x_t)$); in addition, a smoothing effect can be observed (particularly for very small and large values of $x_{1t}$). The informative covariates were selected in all cases, while the noninformative ones were — on average — selected in 11.2% of the cases (7.4% for $\theta_{1t}^{(s_t)}$ and 15.0% for $\theta_{2t}^{(s_t)}$), which again indicates that the variable selection works quite well but apparently is not very conservative (particularly in the case of $\theta_{2t}^{(s_t)}$, where
the shrinkage effect is considerably smaller than the one for $\theta_{1t}^{(st)}$, the average number of noninformative explanatory variables included in the model is fairly large).

For a given number of boosting iterations, model fitting took — on average — 7.8 minutes per (single) model, which again is quite remarkable considering the fact that it does not only involve variable selection among 100 potential covariates (as in the linear setting) but also results in smooth fits (without relying on a computer-intensive smoothing parameter selection).

5 Energy prices in Spain

To illustrate the suggested approach in a real-data setting, we model the conditional distribution of the daily average price of energy in Spain (in Cents per kWh), $Y_t$, over time. Our aim here is to present a simple case-study that provides some intuition and demonstrates the potential of MS-GAMLSS, which is why we focus on a relatively simple model involving only one explanatory variable, the daily oil price (in Euros per barrel), $x_{1t}$. The data, which are available in the R package MSwM (Sanchez-Espigares and Lopez-Moreno, 2014), cover...
1761 working days between February 1, 2002 and October 31, 2008. As in Section 4.2, we assume a normal distribution for the $Y_t$ and fitted two different 2-state MS-GAMLSS with state-dependent predictors for the conditional mean, $\theta_1^{(st)}$, and the conditional variance, $\theta_2^{(st)}$, considering i) simple linear models (linear model), and ii) P-splines (nonlinear model) as base-learners. The stopping iterations were chosen via 20-fold cross validation over the grid $\Lambda = n_{(1)}^{(1)} \times n_{(2)}^{(1)}$, with $n_{(1)}^{(1)} = n_{(2)}^{(1)} = (25, 50, 100, 200, 400, 800, 1600, 3200)$, which led to the optimal values $n_{(1)}^{(1)} = 100$, $n_{(2)}^{(1)} = 200$ (linear model) and $n_{(1)}^{(2)} = 1600$, $n_{(2)}^{(2)} = 200$ (nonlinear model). For the chosen stopping iterations, the computation times were 0.4 minutes (linear model) and 12.9 minutes (nonlinear model).

The off-diagonal t.p.m. entries were estimated as $\hat{\gamma}_{12} = 0.017$, $\hat{\gamma}_{21} = 0.016$ (linear model) and $\hat{\gamma}_{12} = 0.020$, $\hat{\gamma}_{21} = 0.018$ (nonlinear model), which in both cases indicates high persistence within the states (according to the fitted models, the average dwell-times within a state were — depending on the model and the state — between 50 and 62.5 days). The estimated state-dependent distributions, as well as the locally decoded time series of the daily energy prices, are visualized in Figures 7 and 8 respectively: According to both models, the oil price exhibits a (mostly) positive effect on the conditional mean, which essentially holds for both states. However, the linear model lacks the flexibility to capture the decreasing effect for $x_{1t} \geq 60$ that is revealed by the nonlinear model, which leads to a severe overestimation in that area. The effect on the conditional variance considerably differs across the states: In state 1, the oil price has only a minor effect, whereas in state 2, the conditional variance is strongly affected by the oil price. As in the case of the conditional mean, the effect on the conditional variance clearly has a nonlinear form (the volatility is relatively high for $40 \leq x_{1t} \leq 60$ and relatively low for $60 \leq x_{1t} \leq 40$), which is well-captured by the nonlinear model but not captured by the linear model. The consequence is a severe under- (over-) estimation for $40 \leq x_{1t} \leq 60$ ($40 \geq x_{1t} \geq 60$), as indicated by the quantile curves for the linear model depicted in Figure 7. From an economic point of view, state 1 may be linked to a calm market regime (which implies relatively low prices alongside a moderate volatility). State 2, in contrast, may correspond to a nervous market (which implies relatively high prices alongside a high volatility).
Figure 7: Estimated state-dependent predictors for the mean (horizontal solid lines) for states 1 (blue) and 2 (red) and fitted state-dependent distributions for different values of $x_{1t}$ (vertical solid lines), which were computed based on the estimated state-dependent predictors for the variance. Dashed lines indicate the 0.05, 0.15, 0.25, 0.75, 0.85 and 0.95 quantiles of the fitted state-dependent distributions.

Figure 8: Locally decoded time series of the daily energy prices.

The results clearly demonstrate the potential of MS-GAMLSS: By accounting for the state-switching dynamics in the model formulation, they allow to draw a precise picture of the response distribution at any point in time, which may particularly be useful in applications where the focus lies on short-term forecasting. Furthermore, a precise picture of the entire response distribution (which certainly includes not only the mean, but also
variance and potentially skewness and kurtosis parameters) is crucial when the focus is shifted from the expected value towards the quantiles, which for example is the case in risk measurement and portfolio optimization applications (Acerbi, C. and Tasche, D., 2002): Estimating the value-at-risk of a given investment, for instance, requires the prediction of certain quantiles of the corresponding loss distribution (Rockafellar and Uryasev, 2002), which could potentially be addressed using MS-GAMLSS.

6 Discussion

We have introduced MS-GAMLSS as a novel class of flexible latent-state time series regression models which allows to model different parameters of the response distribution as potentially smooth functions of a given set of explanatory variables. Limitations of gradient boosting, particularly the fact that the design of the algorithm does not allow to compute standard errors for the effect estimates, also apply to the MS-gamboostLSS algorithm. While we have assumed a relatively simple state architecture, the underlying dependence structure could potentially be extended in various ways: i) higher-order Markov chains could be used to allow the states to depend not only on the previous state but on a sequence of multiple previously visited states (Zucchini et al., 2016), ii) semi-Markov state processes could be used to specify arbitrary dwell-time distributions for the states (Langrock and Zucchini, 2011), and iii) hierarchical state processes could be used to infer states at multiple temporal scales (Adam et al., 2017; Leos-Barajas et al., 2017).

Another potential feature of the latter approach is that multiple data streams collected at different time scales could be included in a joint, multivariate MS-GAMLSS, which may particularly be useful in economic applications, where data often tend to be collected on a daily, monthly or quarterly basis.

On a final note, we would like to raise awareness of the fact that the flexibility of MS-GAMLSS can be both a blessing and a curse: In some applications, MS-GAMLSS could potentially be overparameterized, and models as complex as MS-GAMLSS may not be appropriate even if they fit the data well (particularly in the case of short time se-
ries, overfitting may become a severe problem). It is therefore worth mentioning that MS-GAMLSS contain other, nested (i.e. less complex) HMM-type models, e.g. simple HMMs (Zucchini et al., 2016) or Markov-switching (generalized) linear and additive models (Langrock et al., 2017; Langrock et al., 2018). By specifying appropriate base-learners, the MS-gamboostLSS algorithm can be used to fit all these nested special cases: Using intercept-only terms (hence neglecting any covariate dependence), for instance, results in simple HMMs, while using simple linear models or P-splines for the conditional mean and intercept-only terms for the other parameters leads to Markov-switching (generalized) linear and additive models, respectively. Since none of the latter classes of models has been incorporated into the gradient boosting framework yet, the MS-gamboostLSS algorithm, which lies at the core of this work, may provide a promising method for model fitting and variable selection not only in MS-GAMLSS but also in a variety of other HMM-type models.

References

Acerbi, C. & Tasche, D. (2002): Expected shortfall: a natural coherent alternative to value at risk. Economic notes, 31 (2), 379–388.

Adam, T., Leos-Barajas, V., Langrock, R. & van Beest, F.M. (2017): Using hierarchical hidden Markov models for joint inference at multiple temporal scales. Proceedings of the 32nd International Workshop on Statistical Modelling, 2, 181–184.

Baum, L.E., Petrie, T., Soules, G. & Weiss, N. (1970): A maximization technique occurring in the statistical analysis of probabilistic functions of Markov chains. Annals of Mathematical Statistics, 41, 164–171.

Beyerlein, A., Fahrmeir, L., Mansmann, U. & Toschke, A.M. (2008): Alternative regression models to assess increase in childhood BMI. BMC medical research methodology, 8, 59.

Biernacki, C., Celeux, G. & Goveart, G. (2013): Assessing a mixture model for clustering
with the integrated completed likelihood. *IEEE Transactions on pattern analysis and machine intelligence*, **22**, 719–725.

Celeux, G. & Durand, J.-B. (2008): Selecting hidden Markov model state number with cross-validated likelihood. *Computational Statistics*, **23**, 541–564.

Cole, T.J. & Green, P.J. (1992): Smoothing reference centile curves: the LMS method and penalized likelihood. *Statistics in Medicine*, **11**, 1305–1319.

de Castro, M., Cancho, V.G. & Rodrigues, J. (2010): A hands-on approach for fitting long-term survival models under the gamlss framework. *Comput. Methods Prog. Biomed.*, **97**, 168–177.

Dempster, A.P., Laird, N.M. & Rubin, D.B. (1977): Maximum likelihood from incomplete data via the EM algorithm. *Journal of the Royal Statistical Society, Series B*, **39**, 1–38.

de Souza, C.P.E. & Heckman, N.E. (2014): Switching nonparametric regression models. *Journal of Nonparametric Statistics*, **26**, 617–637.

Eilers, P.H.C. & Marx, B.D. (1996): Flexible smoothing with B-splines and penalties. *Statistical Science*, **11**, 89–121.

Fontdecaba, S., Munyoz, M.P., & Sanchez, J.A. (2009): Estimating Markovian Switching Regression Models in R. An application to model energy price in Spain. The R Use R Conference 2009. Rennes, France.

Goldfeld, S.M. & Quandt, R.E. (1973): A Markov model for switching regressions. *Journal of Econometrics*, **1**, 3–16.

Hamilton, J.D. (1989): A new approach to the economic analysis of nonstationary time series and the business cycle. *Econometrica*, **57**, 357—384.

Heller, G.Z., Stasinopoulos M.D., Rigby R.A. & de Jong, P. (2007): Mean and dispersion modeling for policy claims costs. *Scandinavian Actuarial Journal*, **4**, 281—292.
Hofner, B., Mayr, A. & Schmid, M. (2016): gamboostLSS: An R package for model building and variable selection in the GAMLSS framework. *Journal of Statistical Software, 74,* 1–31.

Hudson, I.L. (2010): Interdisciplinary approaches: towards new statistical methods for phenological studies. *Climatic Change,* 100, 143–171.

Langrock, R. & Zucchini, W. (2011): Hidden Markov models with arbitrary state dwell-time distributions. *Computational Statistics and Data Analysis, 55,* 715–724.

Langrock, R., Adam, T., Leos-Barajas, V., Mews, S., Miller, D.L. & Papastamatiou, Y.P. (2018): Spline-based Nonparametric Inference in General State-switching Models. *Statistica Neerlandica,* in press.

Langrock, R., Kneib, T., Glennie, R. & Michelot, T. (2017): Markov-switching generalized additive models. *Statistics and Computing, 27,* 259–270.

Leos-Barajas, V., Gangloff, E.J., Adam, T., Langrock, R., van Beest, F.M., Nabe-Nielsen, J. & Morales, J.M. (2017): Multi-scale modeling of animal movement and general behavior data using hidden Markov models with hierarchical structures. *Journal of Agricultural, Biological and Environmental Statistics, 22,* 232–248.

Mayr, A., Fenske, N., Hofner, B., Kneib, T. & Schmid, M. (2012): Generalized Additive Models for Location, Scale and Shape for High Dimensional Data – A Flexible Approach Based on Boosting. *Journal of the Royal Statistical Society, Series C, 61,* 403–427.

Mayr, A., Binder, H., Gefeller, O. & Schmid, M. (2014): The Evolution of Boosting Algorithms - From Machine Learning to Statistical Modelling. *Methods of Information in Medicine, 53* (6), 419–427.

Mayr, A., Schmid, M., Pfahlberg, A., Uter, W. & Gefeller, O. (2017): A permutation test to analyse systematic bias and random measurement errors of medical devices via boosting location and scale models. *Statistical Methods in Medical Research, 26* (3), 1443–1460.

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Pohle, J., Langrock, R., van Beest, F.M. & Schmidt, N.M. (2017): Selecting the number of states in hidden Markov models — pragmatic solutions illustrated using animal movement. *Journal of Agricultural, Biological and Environmental Statistics*, 22(3), 270–293.

Ridgeway, G. (1999): The state of boosting. *Computing Science and Statistics*, 172–181.

Rigby, R.A. & Stasinopoulos, M.D. (2005): Generalized additive models for location, scale and shape. *Journal of the Royal Statistical Society Series C*, 54, 507–554.

Rockafellar, R.T. & Uryasev, S. (2002): Conditional value-at-risk for general loss distributions. *Journal of Banking & Finance*, 26(7), 1443–1471.

Sanchez-Espigares, J.A. & Lopez-Moreno, A. (2014): MSwM: Fitting Markov-Switching Models. R package version 1.2. [http://CRAN.R-project.org/package=MSwM](http://CRAN.R-project.org/package=MSwM).

Stasinopoulos, M.D., Rigby, R.A., Heller, G.Z., Voudouris, V. & de Bastiani, F. (2017): Flexible Regression and Smoothing: Using GAMLSS in R. Chapman & Hall/CRC, Boca Raton.

Thomas, J., Mayr, A., Bischl, B., Schmid, S., Smith, A. & Hofner, B. (2017): Gradient boosting for distributional regression: faster tuning and improved variable selection via noncyclical updates. *Statistics and Computing*, 1–15.

Villarini, G., Smith, J.A., & Napolitano, F. (2010): Nonstationary modeling of a long record of rainfall and temperature over Rome. Advances in Water Resources. *Advances in Water Resources*, 33, 1256–1267.

Voudouris, V., Stasinopoulos, M.D., Rigby, R. & Di Maio, C. (2011): The ACEGES laboratory for energy policy: Exploring the production of crude oil. *Energy Policy*, 39, 5480–5489.

Welch, L.R. (2003): Hidden Markov models and the Baum-Welch algorithm. *IEEE Information Th. Society Newsletter*, 53, 10–13.
