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**Wind Power Scenario Generation Using a High
Dimensional Nonparametric Framework**

Tese de Doutorado

Thesis presented to the Programa de Pós-graduação em Engenharia Elétrica of PUC-Rio in partial fulfillment of the requirements for the degree of Doutor em Engenharia Elétrica.

Advisor: Prof. Alexandre Street de Aguiar

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Abstract

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Producing probabilistic forecasts of Renewable Generation is a topic of interest in power system applications. In this work, we focus on generating future scenarios of wind power generation. Most time series methods used to produce such forecasts rely on the assumption of Gaussian errors or Gaussian distribution, however applications on power systems deals with nongaussian time series. We develop, in this work, a nonparametric methodology based on Quantile Regression to estimate the conditional distribution function for monthly wind time series. The conditional distribution is formed by connecting an array of quantiles jointly estimated. Two different models are used to estimate the quantiles: (i) the model Quantile Regularized Adaptive LASSO (QRAL) and (ii) the Nonparametric Quantile Regression (NQR) model. The QRAL implements two types of regularization. One is based on the Adaptive LASSO for selecting covariates within each Quantile Regression. The other emphasizes the connection across different quantiles, reflecting the fact that the quantile function should have smooth variation, exploring the similarity of neighbor quantiles. The NQR model allows nonlinear functions of its covariates. Each nonlinear function is a continuous function penalized by its second derivative. A case study with realistic Wind Power data from the Brazilian Northeast compares the with different benchmarks in the literature. The QRAL was able to outperform them in terms of minimizing the Mean Absolute Percentile Error of future scenarios in recovering the historic monthly quantiles. The NQR method is under development.

Keywords

Quantile Regression; Model Identification; Nongaussian time series model; Forecasting;

Resumo

C. Ruas, Marcelo; Street, Alexandre. **Geração de Cenários de Geração de Energia Eólica utilizando um Framework não paramétrico de Alta Dimensão**. Rio de Janeiro, 2018. 33p. Tese de Doutorado – Departamento de Engenharia Elétrica, Pontifícia Universidade Católica do Rio de Janeiro.

Produzir previsões probabilísticas de Recursos Renováveis é um tópico e interesse em aplicações de Sistemas de Energia. Neste trabalho, foca-se em gerar cenários futuros de geração de energia eólica. A maior parte dos métodos de séries temporais utilizados para produzir tais previsões baseia-se na hipótese de erros gaussianos ou distribuição gaussiana; no entanto, as aplicações de interesse deste trabalho são séries temporais não gaussianas. Neste trabalho, desenvolve-se uma metodologia não paramétrica baseada em regressão quantílica para estimar a função de distribuição condicional de séries temporais mensais de produção de energia eólica. A distribuição condicional é formada conectando um vetor de quantis estimados conjuntamente. Dois modelos diferentes são utilizados para estimar os quantis: (i) o modelo Quantile Regularized Adaptive LASSO (QRAL) e (ii) o modelo Nonparametric Quantile Regression (NQR). O QRAL implementa dois tipos de regularização. Um é baseado no Adaptive LASSO para selecionar variáveis explicativas dentro de uma regressão quantílica. O outro enfatiza a conexão entre os diferentes quantis, refletindo o fato de que a função quantílica deve variar suavemente. O modelo NQR permite função não-linear das variáveis explicativas. Cada função não-linear é penalizada pela sua segunda derivada. Um estudo de caso com dados reais de produção de energia eólica compara os métodos propostos com outros métodos referência na literatura. O QRAL obteve uma performance melhor que esses outros métodos com relação a minimização do Erro Percentual Absoluto Médio dos cenários futuros em recuperar os quantis históricos mensais. O método NQR ainda está em desenvolvimento.

Palavras-chave

Regressão Quantílica; Identificação de Modelo; Modelos de séries temporais não gaussianos; Previsão;

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1

Introduction

Renewable energy power is an emergent topic which is demanding attention from the academic community. The installed capacity of renewable energy plants has been increasing in a fast pace and projections point out that wind power alone will account to 18% of global power by 2050 (2). In spite of its virtues, several new challenges are inherent when dealing with such power source, due to its unpredictability. To overcome this lack of certainty, one has to work with many different possibilities of outcome.

New statistical models capable of handling such difficulties are an emerging field in power systems literature (3, 4, 5, 6, 7, 8). The main objective in such literature is to propose new models capable of generating scenarios of renewable generation (RG) which are demanded in (i) energy trading, (ii) unit commitment, (iii) grid expansion planning, and (iv) investment decisions (see (9, 10, 11, 12) and references therein). In stochastic optimization, problems such as Unit Commitment, Economic Dispatch, Transmission Expansion Planning all use scenarios as input. Such scenarios are used to characterize the probability distribution within the optimization under uncertainty framework. When working with robust optimization, bounds for probable ranges of coefficients are needed.

Conventional statistical models are often focused on estimating the conditional mean of a given random variable. By reducing the outcome to a single statistic, important informations about the time series random behavior are lost. In order to account for the process inherent variability it is important to consider probability forecasting. In (13), the commonly used methodologies regarding probabilistic forecasting models is reviewed, splitting them in parametric and nonparametric classes. Main characteristics of **parametric models** are (i) assuming a distribution shape and (ii) low computational costs. The ARIMA-GARCH model, for example, fits the RG series by assuming a distribution *a priori*. On the other hand, **nonparametric models** (i) do not require a distribution to be specified, (ii) needs more data to produce a good approximation and (iii) have a higher computational cost. Popular methods are Quantile Regression (QR), Kernel Density Estimation, Artificial Intelligence or a mix of them. Most time series methods rely on

the assumption of Gaussian errors. However, RG time series such as wind and solar are reported as non-Gaussian (3, 14, 15, 16). To circumvent this problem, the usage of nonparametric methods - which does not rely on assuming any previously assumed distribution - appears as a new alternative.

In order to simulate scenarios, not only the conditional mean is needed, but the whole conditional distribution. For example, if two random variables X_1 and X_2 have the same mean but the distribution of X_2 has fatter tails, then simulations from X_2 will present more extreme values than simulations from X_1 . The knowledge of the scale becomes as important as the knowledge of the location when dealing with producing future scenarios. The procedure used for simulating future scenarios is by drawing, in each period τ , a value for $\tau + 1$ from the estimated conditional distribution function (CDF). Hence, having a good estimate of the CDF is essential to meet the goal in this work.

A possibility for constructing the CDF nonparametrically is by using a sequence of quantile values. By estimating many quantiles on a thin grid of probabilities over the interval $[0, 1]$, one can have as many points as desired from an estimated CDF. The second step would be transforming this set of points into a continuous function by a interpolating method. These quantile values may be estimated by a technique such as Quantile Regression (QR). The seminal work (17) defines QR as it is employed in many works (18, 19, 20, 4, 5, 6, 7, 8). The conditional quantile is the solution of an optimization problem where the sum of the check function (defined formally in the next session) is minimized. Instead of using the classical regression to estimate the conditional mean, QR determines any quantile from the conditional distribution. Applications are enormous, ranging from risk measuring at financial funds (the Value-at-Risk) to a central measure robust to outliers.

In (4, 5, 6, 7, 8), QR is employed to model the conditional distribution of wind power Time Series. An updating quantile regression model is presented by (5). The authors present a modified version of the simplex algorithm to incorporate new observations without restarting the optimization procedure. In (6), the authors build a quantile model from already existent independent wind power forecasts. The approach by (4) is to use QR with a nonparametric methodology. The authors add a penalty term based on the Reproducing Kernel Hilbert Space, which allows a nonlinear relationship between the explanatory variables and the output. This work also develops an on-line learning technique, where the model is easily updated after each new observation. In (8), wind power probabilistic forecasts are made by using QR with a special type of Neural Network (NN) with one hidden layer, called extreme learning

machine. In this setup, each quantile is a different linear combination of the features of the hidden layer. The authors of (21) use the weighted Nadaraya-Watson to estimate the conditional function in the time series.

We propose a nonparametric methodology to estimate the CDF given autoregressive terms, with the goal of generating future scenarios of RG. This methodology is based on interpolating individual quantiles, where each quantile is estimated with Quantile Regression. Instead of having an independent model for each quantile, they are all connected in a single problem. All quantiles are jointly estimated by an unique model, whose aim is to estimate quantiles that would later form a CDF after interpolation. This ensures not only that the estimated CDF preserves monotonicity, but also that it is smooth, increasing the out-of-sample predictive assertivity. In this work, the QR may be estimated using two approaches: Quantile Regularized Adaptive LASSO (QRAL) and Nonparametric Quantile Regression (NQR). In both of them, quantiles are jointly estimated in order to build a more reliable distribution function.

The method QRAL relies on a quantile autoregressive (QAR) framework in the same spirit of (17, 22, 23). Notwithstanding, as an innovation from the referenced works, in order to capture which variables would improve model fit, from a set of relevant ones, we propose the use of a LASSO cost function to select which lags are selected to be included in the model. Regularization is a topic already explored in previous QR works. The work by (24) defines the properties and convergence rates for QR when adding a penalty proportional to the ℓ_1 -norm to perform variable selection, using the same idea as the LASSO (25). The AdaLASSO equivalent to QR has its properties investigated by (26). In this variant, the penalty for each variable has a different weight, and this modification ensures that the oracle property is being respected. In (27, 28), the AdaLASSO is employed to QR with multiple quantile regressions at the same time, using the interquantile dependency to improve the quantile coefficient estimation. As a second innovative feature of this work, we propose the inclusion of a penalization parameter of the second difference of quantile values. We argue that such strategy avoids extreme quantiles to be shrinked to zero as fast as the central ones. Such term acts as a filter to impose coefficient stability for a given covariate across the set of quantiles. For the best of the authors knowledge, no other work has developed a methodology where regularization and estimation of the conditional distribution using QR is carried on at the same time with the objective of generating future scenarios for WPG time series.

On the NQR, nonlinearity is considered as an important feature for the model, despite issues come together with nonparametric statistics. Among

these issues are slower convergence to the true parameters and interpolation not straightforward in high dimension. The advantage of this method relative to the linear model is that it allows a nonlinear function of its covariates. Nonparametric quantile function is extensively discussed in (29), and (?) uses a nonlinear estimator for quantile functions for estimating wind power quantiles.

The objective of this work is, then, to propose new methodologies to address simulating future RG scenarios. These methodologies are nonparametric and build the CDF from an array of jointly estimated quantiles, using a penalty which helps to estimate a more appropriate CDF. Two different forms of estimating quantiles are proposed: using linear models and nonparametric quantile regression. The methodology may be seen as a multiple quantile regression problem that specifies a time series model based on the empirical conditional distribution. The main contributions of this work are:

- A nonparametric methodology to model, from a set of quantile estimations, the conditional distribution of RG time series to produce future scenarios.
- The proposition of two different procedures to jointly estimate quantiles:
 - (i) A linear model that selects the global optimal solution with parsimony both on the selection of covariates as on the quantiles. This methodology is based on the Adaptive LASSO for QR (Linear Programming).
 - (ii) A nonparametric quantile regression model, which has a free functional form, tuned by a penalty on how rough this function may be.
- Regularization techniques applied to an ensemble of quantile functions to estimate the conditional distribution, solving the issue of non-crossing quantiles. On regularizing quantiles, we propose a smoothness on the coefficient value across the sequence of quantiles.

The remaining of this work is organized as follows. In section II, we present the quantile regression framework in which we build both QR methods we use in this work: the linear model and nonparametric. In section III, we discuss how to jointly estimate the methods presented in section II to produce the conditional distribution function. Section IV shows how to estimate the models, as well as computational issues regarding the estimation. In Section V, we present a few controlled studies with simulated data and a final case study using real data from wind power is presented in order to test our methodology. Section VI will conclude this article.

2

Quantile Regression based time series model

Let the α -conditional quantile function of Y for a given value x of the d -dimensional random variable X , i.e., $Q_{Y|X} : [0, 1] \times \mathbb{R}^d \rightarrow \mathbb{R}$, can be defined as

$$Q_{Y|X}(\alpha, x) = F_{Y|X=x}^{-1}(\alpha) = \inf\{y : F_{Y|X=x}(y) \geq \alpha\}. \quad (2-1)$$

The Conditional Quantile Function Q is the inverse of the Distribution Function F , and represents the smallest value y for which the distribution function is greater than a given probability α .

Let ρ be the check function

$$\rho_\alpha(x) = \begin{cases} \alpha x & \text{if } x \geq 0 \\ (1 - \alpha)x & \text{if } x < 0 \end{cases}. \quad (2-2)$$

The quantile function for a given finite sample $\{y_t, x_t\}_{t \in T}$, where T is the set of time indexes, and a given probability α is the solution of minimizing the loss function $L_\alpha(\cdot)$:

$$\hat{Q}_{Y|X}(\alpha, \cdot) \in \arg \min_{q \in \mathcal{Q}} L_\alpha(q) = \sum_{t \in T} \rho_\alpha(y_t - q(x_t)). \quad (2-3)$$

For Inference on Quantile Regression and finite sample properties, see the Chapter 3 on (23). The α -quantile function $q(\cdot)$ belongs to a function space \mathcal{Q} . We might have different assumptions for space \mathcal{Q} , depending on the type of function we want to find for q . A few properties, however, must be achieved by our choice of space, such as being continuous and having limited first derivative. In this work, we consider the following two cases:

1. \mathcal{Q} is a linear function space such that $q_\alpha(x_t) = \beta_0 + \beta^T x_t$;
2. \mathcal{Q} is a space of continuous functions with limited first and second derivatives.

2.1

Linear Model

The linear model presumes that the α -quantile function is a linear function of its regressors:

$$q_\alpha(x_t) = \beta_0 + \beta^T x_t.$$

When dealing with many candidates of covariates, one has to deal with the problem of selecting the relevant ones out of a set of candidates which improve model fit. In practice, it means that some coefficients from the vector $\beta = [\beta_1 \cdots \beta_p]$ might assume zero value. There are many ways of selecting a subset of variables among the available options. A classical approach for this problem is the Stepwise algorithm (30), (31), (25), which includes variables in sequence.

A popular way of variable selection which fits on a linear programming context are the LASSO/AdaLASSO techniques, which consists in penalizing the ℓ_1 -norm. Besides shrinking coefficients towards zero, it has also the capability of effectively pushing coefficients to zero (an effect that ridge regression cannot achieve (25)). The usage of LASSO and AdaLASSO in QR context is the topic of study in (32, 26, 24, 27, 28). We refer to the reader the work from (24), where it is possible to find specific properties and convergence rates when using the LASSO to perform model selection in a quantile regression framework.

Regarding the penalization parameter λ , which dictates the shrinkage magnitude of the linear coefficients, the level of parsimony of the model can be defined by the user through such quantity. This is due to the fact that higher values of λ means less variables selected to be non-zero.

The single α -quantile AdaLASSO is estimated by the following optimization problem:

$$\min_{\beta_0, \beta} \sum_{t \in T} \rho_\alpha(y_t - (\beta_0 + \sum_{p \in P} \beta_p x_{tp})) + \lambda \sum_{p \in P} w_p |\beta_p|. \quad (2-4)$$

What differs the AdaLASSO from the LASSO is the inclusion of the term w_p . Suppose the model (2-4) is estimated with all $w_p = 1$, the output of the optimization problem are coefficients of LASSO β_p^L . The AdaLASSO coefficients β_p^{AL} are obtained when solving the same optimization problem while letting $w_p = 1/|\beta_p^L|$.

2.2

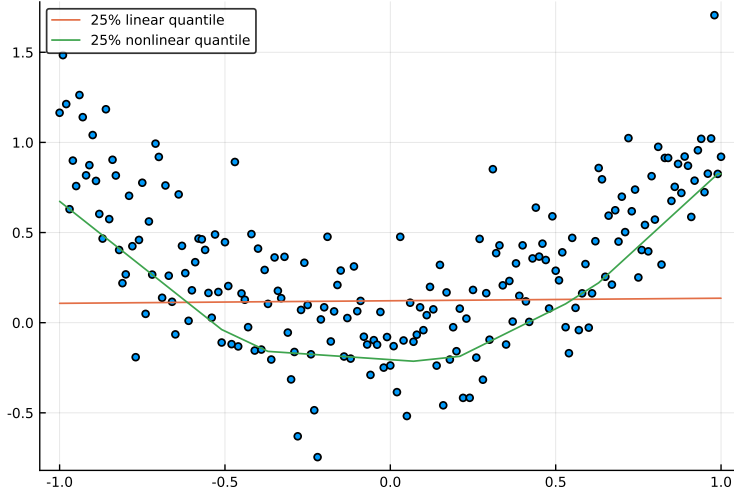


Figure 2.1: Calculating the 25% quantile with both methodologies when there is a nonlinear relationship between x and y . While the linear estimator fails to estimate the conditional quantile, the nonlinear estimator is able to capture the quadratic dependency.

Nonparametric Quantile Regression

Fitting a linear estimator for the QR is less attractive when nonlinearity is present in the quantile functions. In Figure 2.1, a nonlinear relationship between variables x and y is presented, where $y = x^2 + \text{error}$. When using a linear estimator for this type of relation, this estimator underestimates the quantile for a chunk of data while overestimating for the other chunk. In cases such as this, a nonlinear estimator for the quantiles produces better results. Comparing both quantile estimator, it is clear that the nonparametric is capable of capturing the nonlinearity on the relationship, while the linear model can only capture linear relationships.

A nonlinear estimator is built by allowing the quantile function $q(\cdot)$ to freely adjust to the data. The only required aspects for q are being continuous and having limited first and second derivatives. In order to accomplish this, we introduce a Nonparametric Quantile Autoregressive model with a ℓ_1 -penalty term on both the first and second derivatives, represented by their discrete approximation $D^1 q_t$ and $D^2 q_t$ on equations (2-5) and (2-6), respectively, presented below:

$$D_{x_t}^1 q_t = \frac{q_{t+1} - q_t}{x_{t+1} - x_t}, \quad (2-5)$$

$$D_{x_t}^2 q_t = \frac{\left(\frac{q_{t+1} - q_t}{x_{t+1} - x_t} \right) - \left(\frac{q_t - q_{t-1}}{x_t - x_{t-1}} \right)}{x_{t+1} - x_{t-1}}. \quad (2-6)$$

Let $\{\tilde{y}_t\}_{t=1}^n$ be the sequence of observations in time t and let \tilde{x}_t be the p -lagged time series of \tilde{y}_t , such that $\tilde{x}_t = L^p(\tilde{y}_t)$, where L is the lag operator. Matching each observation \tilde{y}_t with its p -lagged correspondent \tilde{x}_t produces

$n - p$ pairs $\{(\tilde{y}_t, \tilde{x}_t)\}_{t=p+1}^n$ (note that the first p observations of y_t must be discarded). When the sequence of observations of x are reorder in such a way that they are in growing order

$$\tilde{x}^{(p+1)} \leq \tilde{x}^{(p+2)} \leq \dots \leq \tilde{x}^{(n)},$$

the new sequences can be defined $\{x_i\}_{i=1}^{n-p} = \{\tilde{x}^{(t)}\}_{t=p+1}^n$ and $\{y_i\}_{i=1}^{n-p} = \{\tilde{y}^{(t)}\}_{t=p+1}^n$, where $T' = \{2, \dots, n - p - 1\}$. The optimization model to estimate the α -quantile nonparametrically is as follows:

$$\begin{aligned} \hat{q}_\alpha(x_t) = \arg \min_{q_t} & \sum_{t \in T'} \rho_\alpha(y - q_t) \\ & + \lambda_1 \sum_{t \in T'} |D_{x_t}^1 q_t| + \lambda_2 \sum_{t \in T'} |D_{x_t}^2 q_t|. \end{aligned} \quad (2-7)$$

The purpose of the filters, then, is to control the amount of variation for the estimator $q_\alpha(x_t)$. When no penalty is employed, the estimated quantile always match the observations $q_{tj} = y_t$, for any given α . On the other hand, when $\lambda_2 \rightarrow \infty$, the estimator approaches the linear quantile regression.

3

Conditional Distribution based on Quantile Regression for Time Series

In the previous section, we presented two methods for estimating a single α -quantile by using QR. However, to build a CDF from an array of quantile, we propose to jointly estimate them, in order to explore the connection across different quantiles.

Let the finite discretization of the interval $[0, 1]$ be composed of a sequence of probabilities $0 < \alpha_1 < \alpha_2 < \dots < \alpha_{|J|} < 1$ and denote as A the set $A = \{\alpha_j \mid j \in J\}$, where J is an index set for the probabilities α . The α -quantiles are, from this point forward, indexed by j , to account for the different models that are simultaneously estimated. A property that must be respected is the monotonicity of the Quantile function Q , such that $q_{\alpha_1} \leq q_{\alpha_2} \leq \dots \leq q_{\alpha_{|J|}}$. The sequence of quantiles define a continuous quantile function after interpolation, and finally a CDF after inverting the estimated quantile function.

The following sections present how to jointly estimate quantiles through QR for each one of the two methods.

3.1

Linear Model

As we are interested on the conditional distribution as a whole, we estimate multiple quantiles at once. In order to produce a coherent distribution function, the output of the problem must respect certain properties, such as being monotone increasing. Besides that, one can expect that the value of similar quantiles be produced by similar models. If the coefficient of a given p covariate changes too abruptly with respect to a change on the probability α , there is a high probability that the estimation did not produce good results rather than this noise belonging to the true model. In order to correct this much common behavior in QR estimation, we introduce a second derivative filter, given by the discrete approximation shown below:

$$D_{\alpha_j}^2 \beta_{pj} := \frac{\left(\frac{\beta_{p,j+1} - \beta_{pj}}{\alpha_{j+1} - \alpha_j} \right) - \left(\frac{\beta_{p,j} - \beta_{p,j-1}}{\alpha_j - \alpha_{j-1}} \right)}{\alpha_{j+1} - \alpha_{j-1}}. \quad (3-1)$$

With this approach, one can keep track on the crossing quantiles issue as well as using a interquantile structure as a strategy to reduce noise on estimation. The works by (27, 28) also use multiple quantile regressions at once and make use of interquantile similarities to produce regularization on the quantiles. In (27), the author uses the norm $\|\beta\|_{1\infty} = \sum_{p=1}^{|P|} \max\{|\beta_j^{(k)}|\}$ as penalization. Such penalization is imposed on the maximum value among all quantiles for a given covariate. This idea is extended by (28), that uses a fused AdaLASSO mixing the LASSO penalization with the absolute interquantile difference.

The statistical model **Quantile Regularized Adaptive LASSO (QRAL)** is defined by the vector of coefficients β_0 and the matrix of size $|P| \times |J|$ of regressor coefficients β_{pj} . These coefficients are the solution from the minimization problem given below:

$$\min_{\beta_{0j}, \beta_j} \sum_{j \in J} \left(\sum_{t \in T} \rho_{\alpha_j}(y_t - (\beta_{0j} + \beta_j^T x_t)) + \lambda \sum_{p \in P} w_{pj}^\delta |\beta_{pj}| \right) + \gamma \sum_{p \in P} \sum_{j \in J'} |D_{\alpha_j}^2 \beta_{pj}|, \quad (3-2)$$

subject to

$$\beta_{0j} + \beta_j^T x_t \leq \beta_{0,j+1} + \beta_{j+1}^T x_t, \quad \forall t \in T, \forall j \in J_{(-1)}, \quad (3-3)$$

where the weights $w_{pj} = 1/\tilde{\beta}_{pj}$ and $\tilde{\beta}_{pj}$ are the coefficients from the first-step LASSO estimation. The parameter δ is an exponential parameter usually set to 1. The sum of absolute values that compose the second derivative filter $\sum_{j \in J'} \sum_{p \in P} |D_{\alpha_j}^2 \beta_{pj}|$ is added on the objective function multiplied by a tuning parameter γ , where the set $J' = \{2, \dots, |J| - 1\}$.

3.2

Nonparametric Quantile Regression

To jointly estimate multiple quantiles, the optimization problem that defines NQR is changed to the following:

$$\min_{q_{tj}} \sum_{j \in J} \left(\sum_{t \in T'} \rho_{\alpha_j}(y - q_{tj}) + \lambda_1 \sum_{t \in T'} |D_{x_t}^1 q_{tj}| + \lambda_2 \sum_{t \in T'} |D_{x_t}^2 q_{tj}| \right), \quad (3-4)$$

$$q_{tj} \leq q_{tj+1}, \quad \forall t \in T, \forall j \in J_{(-1)}, \quad (3-5)$$

where equation (3-5) is a noncrossing constraint and T' is the index set $T' = \{2, \dots, |T| - 1\}$.

Figure 3.1 shows, for realistic data, how the nonlinear estimator can have different degrees of fit on the data. The procedure used to choose the tuning

parameters λ_1 and λ_2 is a topic discussed in the next session, where the cross-validation methodology is presented. The importance of this choice is evident when seeing Figure 3.1, as there is a big tradeoff between bias and variance.

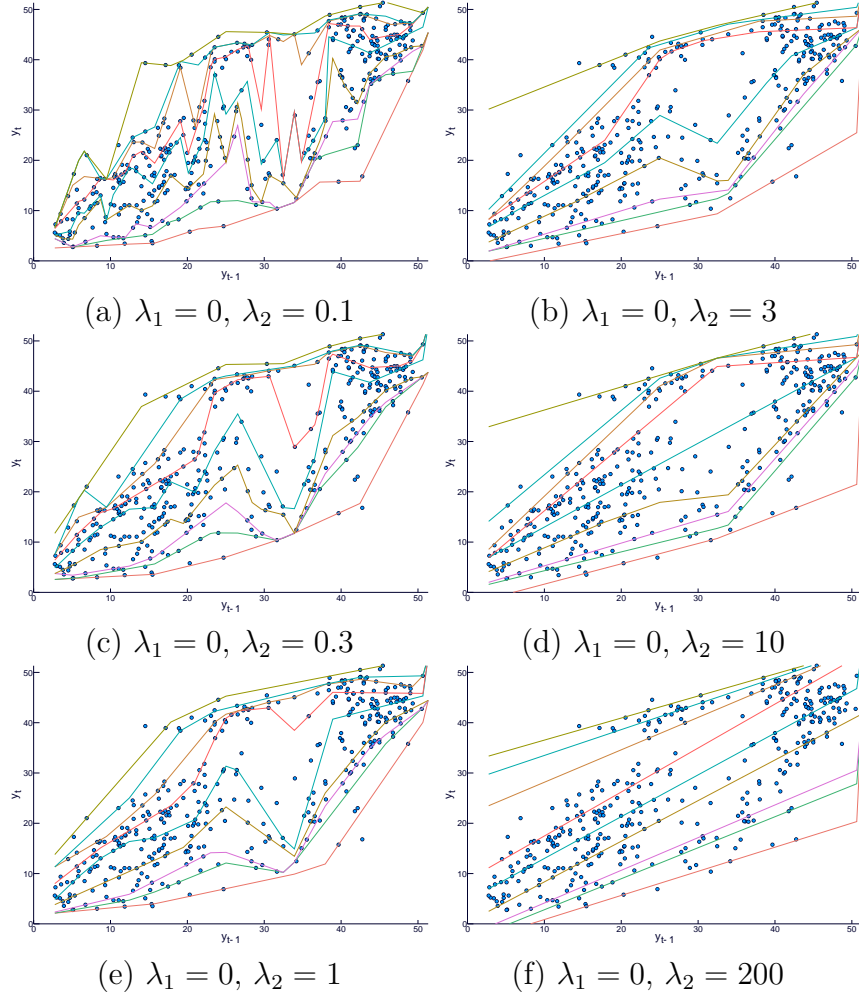


Figure 3.1: Quantile estimations for a few different values of λ_2 . The quantiles represented here are $\alpha = (5\%, 10\%, 25\%, 50\%, 75\%, 90\%, 95\%)$. When $\lambda_2 = 0.1$, on the upper left, estimated quantiles clearly overfit the data. On the other extreme, when $\lambda_2 = 200$, the nonparametric estimator converges to the linear model.

4

Estimation, Evaluation and Simulation procedure

This section presents computational aspects of the estimation, such as presenting the mathematical programming formulation of both the linear and the nonparametric models, presenting the evaluation metric and the cross-validation methodology and the simulation procedure to produce future scenarios of Wind Power. The methodology is implemented in R and Julia languages (relying heavily on the packages JuMP, Gurobi, RCall and Dierckx) and using the Gurobi solver.

4.1

Estimating the QRAL model

The QRAL model, as described in problem (3-2)-(3-3), can be implemented as a linear programming problem as shown below:

$$\begin{aligned} \min_{\beta_0, \beta, \varepsilon_{tj}^+, \varepsilon_{tj}^-, \xi_{pj}^+, \xi_{pj}^-, D2_{pj}^+, D2_{pj}^-} & \sum_{j \in J} \sum_{t \in T} (\alpha_j \varepsilon_{tj}^+ + (1 - \alpha_j) \varepsilon_{tj}^-) \\ & + \lambda \sum_{p \in P} \sum_{j \in J} w_{pj} (\xi_{pj}^+ + \xi_{pj}^-) + \gamma \sum_{p \in P} \sum_{j \in J'} (D2_{pj}^+ + D2_{pj}^-) \end{aligned} \quad (4-1)$$

subject to

$$\varepsilon_{tj}^+ - \varepsilon_{tj}^- = y_t - \beta_{0j} - \beta_j^T x_t, \quad \forall t \in T, \forall j \in J, \quad (4-2)$$

$$\xi_{pj}^+ - \xi_{pj}^- = \beta_{pj}, \quad \forall p \in P, \forall j \in J \quad (4-3)$$

$$D2_{pj}^+ - D2_{pj}^- = \frac{\left(\frac{\beta_{p,j+1} - \beta_{pj}}{\alpha_{j+1} - \alpha_j} \right) - \left(\frac{\beta_{p,j} - \beta_{p,j-1}}{\alpha_j - \alpha_{j-1}} \right)}{\alpha_{j+1} - \alpha_{j-1}}, \quad \forall p \in P, \forall j \in J', \quad (4-4)$$

$$\beta_{0j} + \beta_j^T x_t \leq \beta_{0,j+1} + \beta_{j+1}^T x_t, \quad \forall t \in T, \forall j \in J_{(-1)}, \quad (4-5)$$

$$\varepsilon_{tj}^+, \varepsilon_{tj}^- \geq 0, \quad \forall t \in T, \forall j \in J, \quad (4-6)$$

$$\xi_{pj}^+, \xi_{pj}^- \geq 0, \quad \forall p \in P, \forall j \in J, \quad (4-7)$$

$$D2_{pj}^+, D2_{pj}^- \geq 0, \quad \forall p \in P, \forall j \in J', \quad (4-8)$$

where $J_{(-1)} = \{2, \dots, |J|\}$ is the set which contains all indexes but the first and $J' = \{2, \dots, |J| - 1\}$ is the set which contains all indexes but the first and the last. Variables ε_t^+ and ε_t^- represent the quantities $|y - q(\cdot)|^+$ and $|y - q(\cdot)|^-$, respectively. The first line on the objective function represents the

sum of the check function over all j : $\rho_{\alpha_j}(y - q(\cdot)) = \alpha_j \varepsilon_{tj}^+ + (1 - \alpha_j) \varepsilon_{tj}^-$. The constraint (4-5) assures that the quantile function be monotonic by forcing that, for every x_t and α_j -quantile, $q_{\alpha_j}(x_t) \leq q_{\alpha_{j+1}}(x_t)$. The second derivative term $D_{\alpha_j}^2 \beta_j$ is implemented on the optimization problem by adding a penalty on the objective function to penalize its absolute value, modeled as the sum of auxiliary variables $D_{pj}^+ + D_{pj}^-$. The tuning parameter γ controls how rough the sequence $\{\beta_{pj}\}_{j \in J}$ can be, for a given p .

4.2

Estimating the NQR model

The model presented in equations (3-4)-(3-5) can be rewritten as a LP problem as shown bellow:

$$\begin{aligned} \min_{q_{tj}, \varepsilon_{tj}^+, \varepsilon_{tj}^-, D1_{pj}^+, D1_{pj}^-, D2_{pj}^+, D2_{pj}^-} \quad & \sum_{j \in J} \sum_{t \in T'} \left(\alpha_j \varepsilon_{tj}^+ + (1 - \alpha_j) \varepsilon_{tj}^- \right) \\ & + \lambda_1 \sum_{t \in T'} (D1_{tj}^+ + D1_{tj}^-) + \lambda_2 \sum_{t \in T'} (D2_{tj}^+ + D2_{tj}^-) \end{aligned} \quad (4-9)$$

$$\text{subject to} \quad (4-10)$$

$$\varepsilon_{tj}^+ - \varepsilon_{tj}^- = y_t - q_{tj}, \quad \forall t \in T', \forall j \in J, \quad (4-11)$$

$$D1_{tj}^+ - D1_{tj}^- = \frac{q_{t+1,j} - q_{tj}}{x_{t+1} - x_t}, \quad \forall t \in T', \forall j \in J, \quad (4-12)$$

$$D2_{tj}^+ - D2_{tj}^- = \frac{\left(\frac{q_{t+1,j} - q_{tj}}{x_{t+1} - x_t} \right) - \left(\frac{q_{tj} - q_{t-1,j}}{x_t - x_{t-1}} \right)}{x_{t+1} - x_{t-1}}. \quad \forall t \in T', \forall j \in J, \quad (4-13)$$

$$\varepsilon_{tj}^+, \varepsilon_{tj}^-, D1_{tj}^+, D1_{tj}^-, D2_{tj}^+, D2_{tj}^- \geq 0, \quad \forall t \in T, \forall j \in J, \quad (4-14)$$

$$q_{tj} \leq q_{tj+1}, \quad \forall t \in T, \forall j \in J_{(-1)}, \quad (4-15)$$

where equation 4-15 is the noncrossing constraint. $D1_{tj}^+$ and $D1_{tj}^-$ are auxiliary variables whose sum represent the absolute value of the first derivative of q_t , $|D_{x_t}^1 q_t|$, while $D2_{tj}^+ + D2_{tj}^-$ implement the absolute value of its second derivative $|D_{x_t}^2 q_t|$.

The output of this optimization problem is a sequence of ordered points $\{(x_t, q_{tj})\}_{t \in T}$, for all $j \in J$. The next step is to interpolate these points in order to provide an estimation for any other value of x_t . To address this issue, we propose using a linear interpolation. Note that q_{tj} is a variable that represents only one point of the α_j -quantile function $q_{\alpha_j}(x_t)$.

The quantile estimation is done for different values of λ_2 . By using different levels of penalization on the second difference, the estimation can be more or less adaptive to the fluctuation. It is important to notice that the usage of the ℓ_1 -norm as penalty leads to a piecewise linear solution q_{tj} . Figure 3.1 shows the quantile estimation for a few different values of λ_2 .

4.3

Evaluation Metric

In this section, we present the metric for which the model fit can be evaluated. From this metric, we show two different forms - information criteria and cross validation - to determine the best tuning parameters λ and γ .

In order to evaluate our predictions, we need to define an error metric. The minimization of this error metric is the objective in estimating the statistical model. As conditional distribution is the focus in this paper, we use a performance measurement which emphasizes the correctness across quantiles. Depending on the application, it might be interesting to put different weights on different quantiles. In this work, however, we will treat every quantile as equals concerning the error measure. The chosen error function is Mean Absolute Percentage Error (MAPE), defined by

$$MAPE^{\alpha_j} = \frac{1}{|J|} \frac{1}{|T|} \sum_{t \in T} \sum_{j \in J} \left| \frac{q_t^{\alpha_j} - y_t^{\alpha_j}}{q_t^{\alpha_j}} \right|. \quad (4-16)$$

where $q_t^{\alpha_j}$ is the α -quantile from the data (in the case study, we use the monthly distribution as a good enough approximation of the true quantile, as RG series such as wind power are stationary) and $y_t^{\alpha_j}$ is the α -quantile from these scenarios. This function has the advantage of penalizing error proportionally to the quantile value it is estimating.

4.4

Time-series Cross Validation

Estimating the QRAL involves the use of parameters λ and γ , which should be known *a priori*. In statistics and machine learning, a popular technique is using Cross-validation (CV) to select the best set of parameters from the range of possibilities. How to select their values among this range is a crucial point in our methodology, as the estimated coefficients vary considerably with respect to parameter choice.

Out of the different possible implementations of CV, we use the \mathcal{K} -fold CV. It consists in first partitioning the dataset in \mathcal{K} equally sized sets, which are the \mathcal{K} folds. For each fold $k \in \{1, \dots, \mathcal{K}\}$, the remaining $\mathcal{K} - 1$ folds are used to estimate the model using parameter θ (for the QRAL model, $\theta = [\gamma \ \lambda]^T$) and predicting the values in fold k . The error function $MAPE_\theta^\alpha$ measures the result of this prediction. So, the CV error is given by the sum of all folds and all quantiles, for a given parameter θ

$$CV(\theta) = \sum_{k \in \mathcal{K}} \sum_{j \in J} MAPE_\theta^\alpha.$$

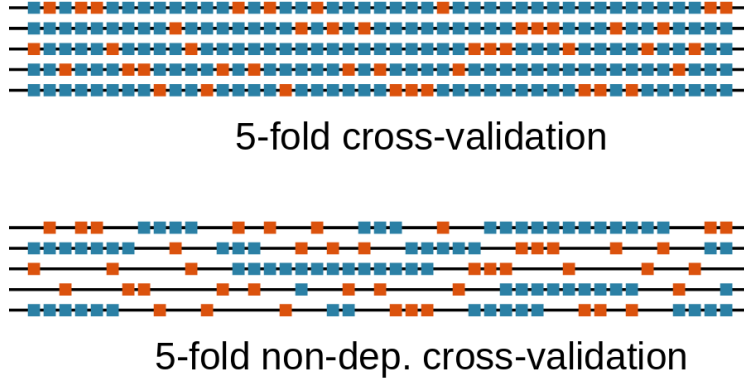


Figure 4.1: \mathcal{K} -fold CV and \mathcal{K} -fold with non-dependent data. Observations in blue are used to estimation and in orange for evaluation. Note that non-dependent data does not use all dataset in each fold. Image from (1).

The optimum parameter θ_{CV}^* , according to this methodology, is the value of θ which minimizes the CV error

$$\theta_{CV}^* = \arg \min_{\theta} CV(\theta). \quad (4-17)$$

The usage of CV is not straightforward when data is dependent, which is the case of time series. As it is time dependent, one can be interested in using either all observations or to take the dependency away to do not interfere on the estimation. The works (1) and (33) deals specifically with the usage of CV in a time series context. They provide tests with both \mathcal{K} -fold CV and \mathcal{K} -fold with non-dependent data. Both schemes are shown of Figure 4.1. In both settings, the training data is randomly split into a collection of sets S_k , forming a \mathcal{K} size partition. Each of these S_k is used as test set, while the rest is used to estimate coefficients which will be used to predict values of S_k . As there are \mathcal{K} folds, this procedure is done \mathcal{K} times. So, for a given vector of tuning parameter θ , the CV score is given by the sum of the error function for each fold. As the CV score is nonconvex, the optimization in (4-17) is done by iterating over a sequence of values in a thin grid and choosing the smallest one.

4.5

Scenario generation

This section presents how to generate future scenarios of time series y_t from the estimated coefficients from a QR model. To produce S different future scenarios $\{\hat{y}_t\}_{t=|T|+1}^{|T|+K}$, we use the following procedure:

Procedure for simulating S future scenarios of $\{y_t\}$

1. Estimate the QR model using one of the methodologies described on section 2:
 - QRAL: solve the QRAL optimization problem defined in equation (4-1)-(4-8). A sequence of coefficients $\{\hat{\beta}_{0j}\}_{j \in J}$ and $\{\hat{\beta}_j\}_{j \in J}$ are the output from this problem.
 - NQR: solve optimization problem (4-9)-(4-15). The output of this problem is a sequence of values $\{\hat{q}_{tj}\}_{t \in T}$ for each α_j -quantile.
 2. Initialize time index $\tau = |T| + 1$.
 3. For each scenario $s \in S$, do
 - (a) Let $x_{\tau,s} = [y_{\tau-1,s}, \dots, y_{\tau-12,s}]$ be the vector of explanatory variables, used as input to predict the conditional distribution function in time τ and scenario s .
 - (b) Let $\tilde{Q}_{y_{\tau}|X} : A \times \mathbb{R}^d \rightarrow \mathbb{R}$ be the discrete quantile function. Its values are mapped according to the chosen QR method:
 - QRAL: $\tilde{Q}_{y_{\tau,s}|X}(\alpha_j, x_{\tau,s}) \leftarrow \hat{\beta}_{0j} + \hat{\beta}_j^T x_{\tau,s}$, for all $j \in J$.
 - NQR: Obtain a continuous quantile function $\bar{q}_{\alpha_j}(\cdot)$ by interpolating the sequence of values $\{\hat{q}_{tj}\}_{t \in T}$. Map $\tilde{Q}_{y_{\tau,s}|X}(\alpha_j, x_{\tau,s}) \leftarrow \bar{q}_{\alpha_j}(x_{\tau,s})$, for all $j \in J$.
 - (c) In order to define the continuous function $\hat{Q}_{y_{\tau}|X} : [0, 1] \times \mathbb{R}^d \rightarrow \mathbb{R}$ from $\tilde{Q}_{y_{\tau,s}|X}$, use linear interpolation connecting the points. As $0 < \alpha_1 < \dots < \alpha_{|J|} < 1$, there are no quantile estimates for the intervals $[0, \alpha_1]$ and $[\alpha_{|J|}, 1]$. These gaps are filled by linearly extending the line that connects α_1 to α_2 on the left hand side and extending the line that connects $\alpha_{|J|-1}$ to $\alpha_{|J|}$ on the right hand side until the support $[0, 1]$ is fully mapped.
 - (d) Let U be a random variable with uniform distribution over the interval $[0, 1]$. By using the result of the Probability Integral Transform (PIT), random variable $F_{y_{\tau}}^{-1}(U)$ has the same distribution as y_{τ} . The time series value at time τ and s scenario $y_{\tau,s}$ is built by drawing one random observation of U and applying the transformation of the PIT.
 4. Let $\tau = \tau + 1$. If $\tau > K$, then stop. Else, go back to step 3) .
-

5

Case Studies

5.1

Controlled Studies I - Autoregressive Process

Firstly, the performance of QRAL methodology is evaluated by simulating a widely used autoregressive process and in the sequel estimating the QRAL framework to evaluate if it is capable to recover the parameters fixed at the beginning. The aforementioned autoregressive process is set as

$$y_t = \beta_1 y_{t-1} + \varepsilon_t, \quad \varepsilon_t \sim N(0, 1), \quad (5-1)$$

with length 400 and $\beta_1 = 0.3$. This value was chosen due to the fact that the sample size of RG time series have such length in general.

Three different methods were employed to estimate the process given by (5-1):

1. **Quantile Regularized Adaptive LASSO (QRAL)**, which estimates one different model for each quantile $Q_{y_t|X}(\alpha, \cdot)$, for all $j \in J$. In practice, it means that each coefficient β_{1j} is estimated with regularization on each quantile.
2. **Quantile Regression as Koenker (QRK)** as originally proposed by (17), where each coefficient β_{1j} is estimated using QR.
3. A simple **Autoregressive (AR)** process.

After simulate 1000 different time series given by Equation (5-1), β_{1j} was estimated for each one of the aforementioned models. Regarding parameter γ (see Eq. (4-1)-(4-8)) it was estimated using CV, as described in section 4.4. Since in this experiment the model has only one lag, model selection will not be evaluated, hence $\lambda = 0$.

The main objective of this simulation experiment was to evaluate how our nonparametric methodology can correctly recover the true AR(1) process. The model performance was evaluated by examining how closely the estimated quantiles are from the populational ones. The results for each method are depicted in Figure 5.1, where a boxplot containing the results for the 1000

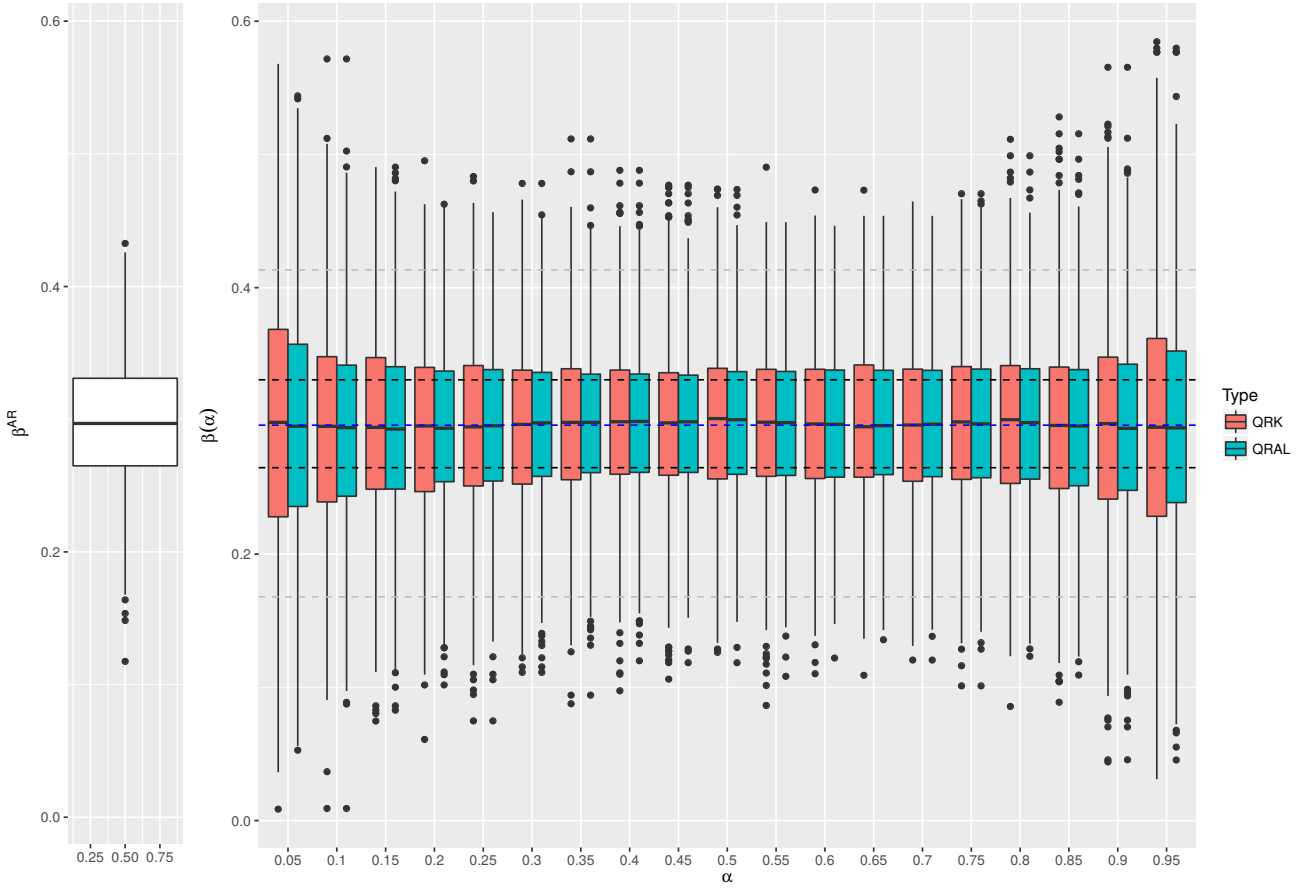


Figure 5.1: Boxplot showing estimated coefficient after 1000 iterations. On the left hand side, the boxplot of the AR(1) coefficient estimation. Note that for the AR(1) the coefficient is equal for all probabilities α . On the right hand side, the boxplot of the regular QR (where $\gamma = 0$) and the QRAL where γ is selected using cross-validation.

simulations is shown. The conclusions from this experiment are: (i) Coefficient estimation errors for the central quantiles are not far from those estimated by the AR; (ii) extreme quantiles are usually harder to estimate, due to having fewer observations; as a consequence, the estimation error increases on the extremes (iii) QRAL has an advantage over QQR in terms of variance of estimators.

5.2

Controlled Studies II - Quantile Autoregressive Process

In the second controlled study, the performance of the QRAL is evaluated in a Quantile Autoregressive Process. While in the first study the time series y_t is generated by a process with a coefficient β_1 constant across quantiles, in this experiment β_1 is a piecewise linear function of α , described graphically on Figure 5.2.

The simulation of a QAR process involves two steps. The first is to

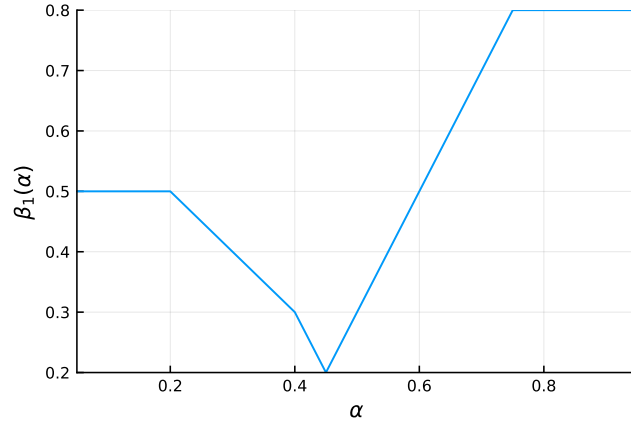


Figure 5.2: Coefficient $\beta_1(\alpha)$ of the Autoregressive term y_{t-1} for generating the QAR process.

determine the values of β_0 from a set of values of $\beta_1(\alpha)$; the latter given as input. These values of β_{0j} are the output of the following optimization problem:

$$\min_{\beta_0} \beta_{0,|J|} - \beta_{0,1} \quad (5-2)$$

$$\text{subject to} \quad (5-3)$$

$$\beta_{0j} + \beta_j^T x_t + h \leq \beta_{0,j+1} + \beta_{j+1}^T x_t, \quad \forall t \in T, \forall j \in J_{(-1)}, \quad (5-4)$$

where h is the minimum distance allowed between two neighbour quantiles. If $\beta(\alpha)$ is constant for an interval and h is set to zero, this group of quantiles would superimpose one another. Once both vectors β_0 and β_1 are defined, the 1-step temporal dynamic of the process can be summarized by Figure 5.3.

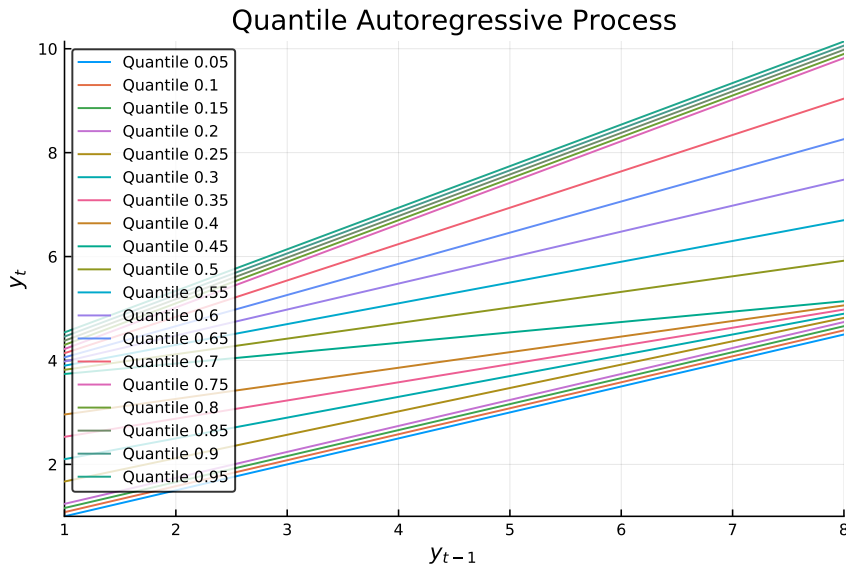


Figure 5.3: Quantiles of y_t vs y_{t-1} . For each given value of y_{t-1} on the x -axis, the curves indicate different levels of quantiles for the values of y_t .

The second step consists in simulating the values of y_t . For a given value

of y_{t-1} , the next term y_t in the time series follows a distribution that can be constructed by the quantiles shown on Figure 5.3.

This controlled study has the same sample setup as the one in the previous section: 1000 random samples of length 400 and the same three methods tested (QRAL, QRK and AR). The objective of this experiment is to test their performance with respect to their error on the estimation of each coefficient. The summary of results is given by Table 5.1, which shows the aggregated value of quadratic error across all $j \in J$. The conclusion from this experiment is that both QR methods are much superior than an Autoregressive process such as a AR(1) when the coefficient β is allowed to change with probability α .

| AR(1) | QR-AdaLASSO | QRK |
|-------|-------------|-------|
| 38.75 | 5.039 | 5.314 |

Table 5.1: Cumulated quadratic error of coefficient estimation for each method after 1000 random samples

5.3

Case Study with realistic data

In this section, the QRAL methodology is tested in generating future scenarios of RG. A real time series of Wind Power is the input for estimating coefficients that are employed to generate scenarios by using the procedure described on section 4.5. The time series is composed of 31 years (from 1981 to 2011) of monthly observations of a wind farm located in the Brazilian northeast, measured in Megawatts. The yearly series is shown on Figure 5.4.

The last 4 years of this period is leaved as out-of-sample test data. Six different methods are used to generate scenarios: QR-LASSO (Quantile Regularized LASSO), QRAL, QRK, LASSO (original LASSO for QR), AdaLASSO (original AdaLASSO for QR) and SARIMA. The estimated coefficients for the QR based methods are presented on Figure 5.5. The second derivative filter acts reducing the noise, and its effect can be seen clearly when comparing the estimated coefficients of QR-LASSO with the LASSO and the QRAL with the AdaLASSO.

The accuracy of the generated scenarios - considering the MAPE metric - in recovering the historic quantiles for each month is the metric used for evaluation. These results are shown on Table 5.2. The QRAL is the method that produced the scenarios with the smaller errors.

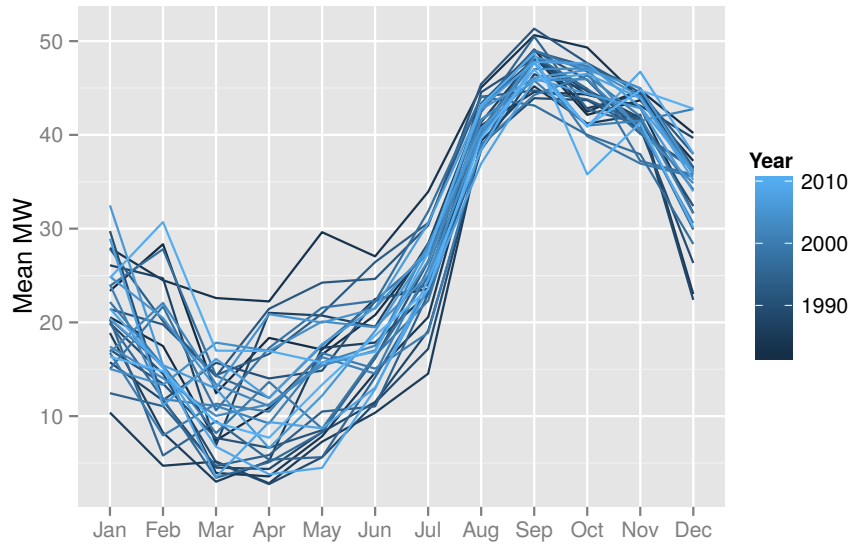


Figure 5.4: Icaraizinho yearly data. Each serie consists of monthly observations for each year.

| QR-LASSO | QR-AdaLASSO | QRK | LASSO | AdaLASSO | SARIMA |
|----------|-------------|-------|-------|----------|--------|
| 6.809 | 3.653 | 3.940 | 6.282 | 4.653 | 5.834 |

Table 5.2: Cumulated MAPE across all α_j quantiles

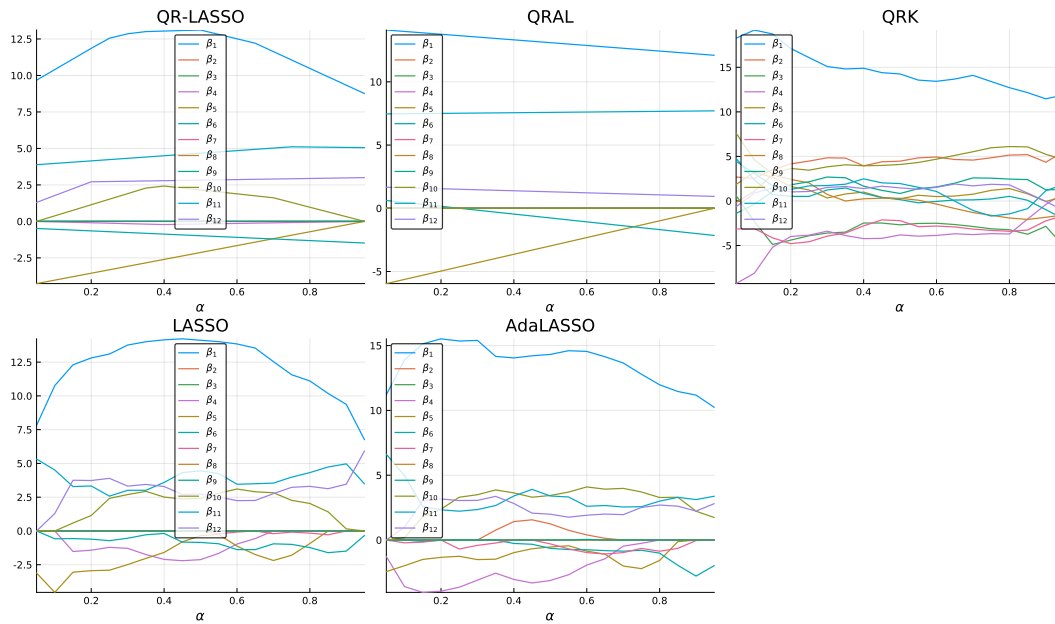


Figure 5.5: Estimated coefficients for each QR based methods. Each line represents the coefficient function β_p for a given covariate y_{t-p} .

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