An Object-oriented Framework for Quantile-based Spectral Analysis and a Reference Implementation in R: The quantspec Package

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Abstract

Quantile-based spectral approaches to the analysis of time series have recently attracted a lot of attention. In several publications the advantages of copula-based measures for serial dependence over the traditional moment-based ones have been discussed and two different types of estimators were proposed. The asymptotic properties of these estimators were subject to many a detailed analysis with the results published in several scientific papers. In this paper aspects of their systematic computation are investigated. An extensible framework is developed and documented using object-oriented models. As a comprehensive reference implementation the R package quantspec was made available and the contribution in this paper includes a tutorial, with worked examples. A reader who is already familiar with quantile-based spectral analysis and whose primary interest is not the design of the quantspec package, but how to use it, can read the tutorial and worked examples (Sections 3 and 4) independently.

This introduction to the R package **quantspec** is a (slightly) modified version of a paper (to be) submitted to the *Journal of Statistical Software*.

Keywords: time series, spectral analysis, periodogram, quantile regression, copulas, ranks, R, **quantspec**, framework, object-oriented design.

1. A short introduction to quantile-based spectral analysis

1.1. Laplace and copula cumulants and their spectral representation

While traditionally the analysis of serial dependence in a stationary process is based on covariance and correlation functions (or their spectral representations) the objects of interest in quantile-based spectral analysis are the *Laplace cross-covariance kernel*

$$\gamma_k(q_1, q_2) := \text{Cov}\Big(I\{X_t \le q_1\}, I\{X_{t-k} \le q_2\}\Big), \quad q_1, q_2 \in \bar{\mathbb{R}}, \ k \in \mathbb{Z},$$

and the copula cross-covariance kernel

$$\gamma_k^U(\tau_1, \tau_2) := (I\{F(X_t) \le \tau_1\}, I\{F(X_{t-k}) \le \tau_2\}), \quad \tau_1, \tau_2 \in [0, 1], \ k \in \mathbb{Z},$$

where $I\{A\}$ denotes the indicator function of the event $\{A\}$ and F the marginal distribution function (the distribution function of any X_t , due to the assumed stationarity). Obviously these measures always exist without the necessity to make assumptions about moments. Also, when considered as a function with arguments q_1, q_2 or τ_1, τ_2 respectively they provide a much richer picture about the pairwise dependence than would the autocovariances. Another feature that can be quite handy in many applications is the invariance of the copula cross-covariance kernel to monotone transformations, which in particular disentangles the serial features from the marginal features. The full amount of advantages for considering these measures is too extensive to be discussed here in full detail and further arguments are omitted since thorough discussions are already available in Dette, Hallin, Kley, and Volgushev (2013) and Kley, Volgushev, Dette, and Hallin (2014).

Under sumability conditions the Laplace spectral density kernel

$$\mathfrak{f}_{q_1,q_2}(\omega) := \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \gamma_k(q_1, q_2) e^{-ik\omega}, \quad q_1, q_2 \in \overline{\mathbb{R}}, \ \omega \in \mathbb{R},$$
 (1)

and the copula spectral density kernel

$$\mathfrak{f}_{q_{\tau_1}, q_{\tau_2}}(\omega) := \frac{1}{2\pi} \sum_{k = -\infty}^{\infty} \gamma_k^U(q_1, q_2) e^{-ik\omega}, \quad \tau_1, \tau_2 \in [0, 1], \ \omega \in \mathbb{R},$$
 (2)

exist, where $q_{\tau} := F^{-1}(\tau)$. Admitting the representation

$$\gamma_k(q_1, q_2) = \int_{-\pi}^{\pi} e^{ik\omega} \mathfrak{f}_{q_1, q_2}(\omega) d\omega,$$

and a similar representation for $\gamma_k^U(\tau_1, \tau_2)$, they are equivalent to the "time-domain" quantities. Sometimes considering the cumulated Laplace or copula spectral density kernels, which can be defined as

$$\mathfrak{F}_{q_1,q_2}(\omega) := \int_0^\omega \mathfrak{f}_{q_1,q_2}(\lambda) d\lambda, \quad q_1, q_2 \in \bar{\mathbb{R}}, \ \omega \in [0, 2\pi], \tag{3}$$

and

$$\mathfrak{F}_{q_{\tau_1}, q_{\tau_2}}(\omega) := \int_0^\omega \mathfrak{f}_{q_{\tau_1}, q_{\tau_2}}(\lambda) d\lambda, \quad \tau_1, \tau_2 \in [0, 1], \ \omega \in [0, 2\pi], \tag{4}$$

is more convenient.

1.2. Estimators for the quantile-based spectral analysis of time series

The following quantile periodogram statistics can be used for the estimation of the Laplace and copula-spectra defined in Section 1.1. For the upcoming definitions denote by X_0, \ldots, X_{n-1} an observed time series of the process $(X_t)_{t\in\mathbb{Z}}$, and by

$$\hat{F}_n(x) := \sum_{t=0}^{n-1} I\{X_t \le x\}$$

the empirical distribution function of X_0, \ldots, X_{n-1} . Further,

$$\rho_{\tau}(x) := x(\tau - I\{x < 0\}) = (1 - \tau)|x|I\{x < 0\} + \tau|x|I\{x > 0\},$$

denotes the so-called *check function* [cf. Koenker (2005)].

Definition 1 (Quantile-regression based periodograms)

For $\omega \in \mathbb{R}$ and $\tau_1, \tau_2 \in (0,1)$ the Laplace periodogram $\hat{L}_n^{\tau_1,\tau_2}(\omega)$, and the rank-based Laplace periodogram $\hat{L}_{n,R}^{\tau_1,\tau_2}(\omega)$ are defined as

$$\hat{L}_{n}^{\tau_{1},\tau_{2}}(\omega):=(2\pi n)^{-1}\hat{b}_{n}^{q_{1}}(\omega)\hat{b}_{n}^{q_{2}}(-\omega),\quad \hat{L}_{n,R}^{\tau_{1},\tau_{2}}(\omega):=(2\pi n)^{-1}\hat{b}_{n,R}^{\tau_{1}}(\omega)\hat{b}_{n,R}^{\tau_{2}}(-\omega),$$

where, for $\omega \neq 0 \mod \pi$, and $\tau \in (0,1)$,

$$(\hat{a}^{\tau}(\omega), \hat{b}_{n}^{q}(\omega)) := \operatorname{argmin}_{a \in \mathbb{R}, b \in \mathbb{C}} \sum_{t=0}^{n-1} \rho_{\tau}(nX_{t-1} - a - 2\cos(\omega t)\Re b - 2\sin(\omega t)\Im b),$$
 (5)
$$(\hat{a}^{\tau}(\omega), \hat{b}_{n,R}^{\tau}(\omega)) := \operatorname{argmin}_{a \in \mathbb{R}, b \in \mathbb{C}} \sum_{t=0}^{n-1} \rho_{\tau}(n\hat{F}_{n}(X_{t}) - a - 2\cos(\omega t)\Re b - 2\sin(\omega t)\Im b).$$

If $\omega = 0 \mod \pi$, when the regressor that yields the imaginary part of the estimate vanishes, the estimates need to be adapted as follows: for $\omega_{\pi} = 2\pi(j+1/2)$, $j \in \mathbb{Z}$, let

$$(\hat{a}^{\tau}(\omega_{\pi}), \hat{b}_{n}^{q}(\omega_{\pi})) := \operatorname{argmin}_{a \in \mathbb{R}, b \in \mathbb{R}} \sum_{t=0}^{n-1} \rho_{\tau}(nX_{t} - a - \cos(\omega_{\pi}t)b),$$
$$(\hat{a}^{\tau}(\omega_{\pi}), \hat{b}_{n,R}^{\tau}(\omega_{\pi})) := \operatorname{argmin}_{a \in \mathbb{R}, b \in \mathbb{R}} \sum_{t=0}^{n-1} \rho_{\tau}(n\hat{F}_{n}(X_{t}) - a - \cos(\omega_{\pi}t)b).$$

For $\omega \in 2\pi\mathbb{Z}$ an adaptation is also possible [cf. Kley (2014a)], but since it is not required for the definition of the smoothed estimates it is omitted for the sake of brevity.

The Laplace periodograms trace back to Li (2008) who, in a pioneering paper, suggested least absolute deviation estimators in a harmonic linear model. He later extended the approach to arbitrary quantiles Li (2012). Dette *et al.* (2013) introduced the estimator with distinct quantile levels τ_1 and τ_2 (not necessarily equal), and based it on the ranks.

Definition 2 (Periodograms based on clipped time series)

For $\omega \in \mathbb{R}$ and $q_1, q_2 \in \mathbb{R}$, the clipped time-series periodogram is defined as

$$I_n^{q_1,q_2}(\omega) := (2\pi n)^{-1} d_n^{q_1}(\omega) d_n^{q_2}(-\omega), \quad d_n^q(\omega) := \sum_{t=0}^{n-1} I\{X_t \le q\} e^{-i\omega t}.$$

For $\omega \in \mathbb{R}$ and $\tau_1, \tau_2 \in [0,1]$ the copula rank periodogram is defined as

$$I_{n,R}^{\tau_1,\tau_2}(\omega) := (2\pi n)^{-1} d_{n,R}^{\tau_1}(\omega) d_{n,R}^{\tau_2}(-\omega), \quad d_{n,R}^{\tau}(\omega) := \sum_{t=0}^{n-1} I\{\hat{F}_n(X_t) \le \tau\} e^{-\mathrm{i}\omega t}.$$

Note the similarity between all the periodogram-like estimators and the cross-periodograms in multivariate time series analysis [cf., e.g., Brillinger (1975), p. 235]: each periodogram is a product of two frequency representation objects computed at frequencies (ω and $-\omega$) that sum to zero

The estimator based on the discrete Fourier transformation of $I\{\hat{F}_n(X_t) \leq \tau\}$ was introduced by Hagemann (2011), for the special case of $\tau_1 = \tau_2$. The case of distinct quantile levels τ_1

and τ_2 (not necessarily equal) was discussed in Kley et al. (2014), where weak convergence to a Gaussian process is proven.

1.3. Smoothing the quantile periodograms

As in the traditional case the new periodograms are not consistent estimators [cf. the positive variances of the limit distributions in Theorems 3.2 and 3.4 in Dette *et al.* (2013) or Proposition 3.4 in Kley *et al.* (2014)]. To achieve consistency of the estimators we convolve the sequence of periodograms (indexed with the Fourier frequencies) with a sequence of weighting functions W_n . When the weight functions are such that with $n \to \infty$ only the weights in a shrinking neighborhood of zero will be positive, the estimator will be consistent.

The smoothed periodograms are defined as follows:

Definition 3 (Smoothed quantile-regression based periodograms)

For $\omega \in \mathbb{R}$ and $\tau_1, \tau_2 \in (0,1)$ the smoothed Laplace periodogram $\hat{\mathfrak{f}}_n(\tau_1, \tau_2; \omega)$ and smoothed rank-based laplace periodogram $\hat{\mathfrak{f}}_{n,R}(\tau_1, \tau_2; \omega)$ are defined as

$$\hat{\mathfrak{f}}_n(\tau_1, \tau_2; \omega) := \frac{2\pi}{n} \sum_{s=1}^{n-1} W_n(\omega - 2\pi s/n) \hat{L}_n^{\tau_1, \tau_2}(2\pi s/n),$$

$$\hat{\mathfrak{f}}_{n,R}(\tau_1,\tau_2;\omega) := \frac{2\pi}{n} \sum_{s=1}^{n-1} W_n(\omega - 2\pi s/n) \hat{L}_{n,R}^{\tau_1,\tau_2}(2\pi s/n).$$

Definition 4 (Smoothed periodograms based on clipped time series)

For $\omega \in \mathbb{R}$ and $q_1, q_2 \in \mathbb{R}$ the smoothed clipped time series periodogram is defined as

$$\hat{G}_n(q_1, q_2; \omega) := \frac{2\pi}{n} \sum_{s=1}^{n-1} W_n(\omega - 2\pi s/n) I_n^{q_1, q_2}(2\pi s/n).$$

For $\omega \in \mathbb{R}$ and $\tau_1, \tau_2 \in [0, 1]$ the smoothed copula rank periodogram is defined as

$$\hat{G}_{n,R}(\tau_1, \tau_2; \omega) := \frac{2\pi}{n} \sum_{s=1}^{n-1} W_n (\omega - 2\pi s/n) I_{n,R}^{\tau_1, \tau_2}(2\pi s/n).$$

A comprehensive description of all estimators and their asymptotic properties is available in Kley (2014a).

2. Conceptual design of the framework

2.1. An analysis of functional requirements

The **quantspec** software project was triggered by the development of the quantile-based methods for spectral analysis [cf. Section 1, Dette *et al.* (2013) and Kley *et al.* (2014)]. The primary aim has been to make these new methods accessible to a wide range of users.

Before going into the programming-specific details of the project, a conceptual design, non-specific to any specific programming language was developed. By this procedure, additional insight and a thorough documentation of the computational characteristics of quantile-based spectral analysis could be gained. The conceptual design serves as a blueprint for implementations in (possibly) various environments and can easily be transformed into an implementation plan including the details specific to the respective programming environment.

Aiming for a software system that is most flexible in the ways in which it can be used, that can easily be extended in functionality and also for the ease of it's maintenance an object-oriented design was chosen. This type of design also contributes to a structure of the system that can be better understood, both by users and developers. The general structure of the system for performing quantile-based spectral analysis is described using class diagrams of the unified modeling language (UML). In these diagrams, all necessary components and their interrelations are described in a formal manner.

To understand the specification of the framework, recall that in an object-oriented design the components of the system are objects encapsulating both data and behavior of a specific "real-world" entity. The structure of each object can thus be described by a meaningful name (the class name), a collection of data fields (in R these are called slots) and implementations of the behavior (in R these implementations are called methods). In a class diagram each class (i.e., the composite of class name, data files and implemented behavior) is represented as a rectangle subdivided into three blocks. The name of the class is given in the top block, the data fields in the middle block and the methods in the bottom block. Note that in the unified modeling language the data fields and methods are specified in a standardized format. In this format the first symbol is an abbreviation used to specify the visibility of the class member. Here "+" for public and "-" for private members are used, meaning that the member is intended to be seen (and used) from outside the object or from inside the object only, respectively. For a data field the name is then followed by a colon and the type of the field. For a method the parameters are given in parenthesis; optional parameters are denoted by two dots. In the class diagram, relationships between classes are marked as lines connecting them. Currently two different types of relationships are modeled. A line with a triangular shaped tip at one end is used to declare a generalization relationship (sometimes also coined inheritance or "is a" relationship). The class at the end of the line with the triangle is called the superclass or the parent, while the class on the other side is called the subclass or the child. In particular this type of relationship implies that an object that is an instance to the subclass and therefore provides all the subclasses' data fields and methods will also provide the data fields and methods of the superclass (and the superclasses' superclass it there are such, etc.). The second type of relationships used in this framework is that of an aggregation (sometimes called "has a" relationship). A line with a hollow diamond at one end is used to denote this kind of relationship, where objects to the class at the end of the line with the diamond are the ones having objects of the class at the other end of the line as a part of them.

At each end of the line the so-called cardinalities are denoted in the form of two numbers with dots in between them. The left number is the minimum number of objects of that type in the relationship that need to exist, the right number is the maximum number. A star is used to denote an unknown positive integer. If min and max cardinality coincide it is displayed without the dots.

For the class diagrams in this manuscript the classes are arranged in a way such that (whenever possible) generalization relationships are displayed with the superclass on top and the subclasses in the bottom. Aggregations are shown with aggregated classes to the left and/or the right of the class representing "the whole".

A graphical representation of the framework for quantile-based spectral analysis is not given in one holistic diagram, but in two class diagrams that are on display in Figures 1 and 2. The structure of the framework is presented in two, thematically organized class diagrams rather than in one, because the 13 classes and their relations could not be fitted easily onto one page without breaking the above mentioned layout guidelines. On the other hand it was easy to group the classes by two topics.

In the next sections, all classes of the framework and their relations are going to be thoroughly described and motivated.

2.2. The base class QSpecQuantity and its successors

Many of the quantities important for the quantile-based spectral analysis of a stationary time series [i. e., the estimators of Definitions 1–4 and the model quantities (1)–(4)] are of the functional form,

$$Q_b: F \times T_1 \times T_2 \to \mathbb{C}, \quad b = 1, \dots, B$$

where $F \subset \mathbb{R}$ is a set of frequencies [e. g, $F = [0, 2\pi)$] and $T_1, T_2 \subset \overline{\mathbb{R}}$ are sets of levels. To provide a common interface to these objects the abstract class QSpecQuantity was introduced. It's data fields (i. e., the array values, a vector of reals frequencies and a list with two vectors of reals levels), are designed to store the sets

frequencies :=
$$\{\omega_1, \dots, \omega_J\} \subset F$$
,
levels[[1]] := $\{q_{1,1}, \dots, q_{1,K_1}\} \subset T_1$,
levels[[2]] := $\{q_{2,1}, \dots, q_{2,K_2}\} \subset T_2$,

and the family

values :=
$$(Q_b(\omega_j, q_{1,k_1}, q_{2,k_2}))_{j=1,\dots,J;k_1=1,\dots,K_1;k_2=1,\dots,K_2;b=1,\dots,B}$$
.

Note that the handling of a family of B quantile spectral quantities is necessary when bootstrapping replicates are present. The special case of only one function Q can easily be handled by setting B = 1.

There are four classes inheriting the data structure and the method show¹ from the abstract class QSpecQuantity. Two such classes, QuantilePG and SmoothedPG, implement the computation of the various quantile periodograms and smoothed quantile periodograms, respectively. A more detailed description has to include the other related classes and is therefore deferred

¹The function show is used for printing object's of this class, and all superclasses, to the console.

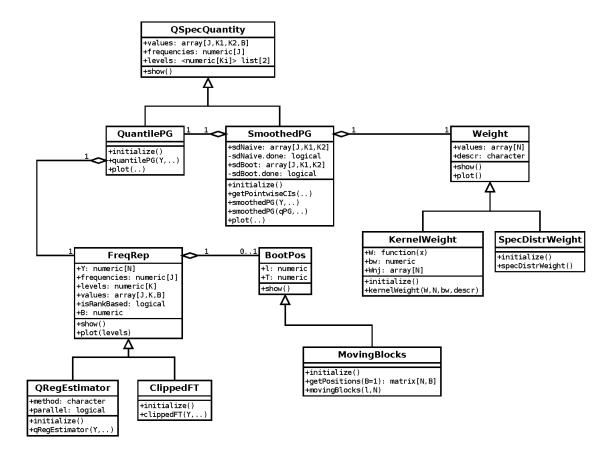


Figure 1: Classes implementing the quantile-based periodograms and smoothed periodograms

to a separate section (i. e., Section 2.3). A graphical representation of the relevant parts of the framework can be seen in Figure 1. The other two of the classes generalizing the abstract class QSpecQuantitiy are referred to by the names QuantileSD and IntegrQuantileSD. These two classes implement the model quantities (1)–(4). The graphical representation can be seen in Figure 2. A detailed description is deferred to Section 2.4.

2.3. Implementation of the quantile-based (smoothed) periodograms

The components relevant to the implementation of the quantile-based spectral statistics are presented in Figure 1. As alluded to in the previous section the two classes QuantilePG and SmoothedPG will do the job, in conjunction with the superclass QSpecQuantity from which they inherit the data structure to store the computed values.

To better understand the implementation surrounding QuantilePG, observe that the quantilebased periodograms defined in Definitions 1 and 2 share the common structure of an outer product (scaled with $(2\pi n)^{-1}$). To compute either one of the four periodograms

$$\hat{L}_{n,R}^{\tau_1,\tau_2}(\omega), \ \hat{L}_{n}^{\tau_1,\tau_2}(\omega), \ I_{n,R}^{\tau_1,\tau_2}(\omega), \quad \tau_1 \in T_1, \ \tau_2 \in T_2, \ \omega \in F,$$

$$I_{n}^{q_1,q_2}(\omega) \quad q_1 \in Q_1, \ q_2 \in Q_2, \ \omega \in F,$$

it suffices to perform the same operation to one of the frequency representation objects

$$\hat{b}_{n,R}^{\tau}(\omega), \ \hat{b}_{n}^{\tau}(\omega), \ d_{n,R}^{\tau}(\omega), \quad \tau \in T_{1} \cup T_{2}, \ \omega \in F,$$

$$d_{n}^{q}(\omega) \quad q \in Q_{1} \cup Q_{2}, \ \omega \in F,$$

$$(6)$$

respectively. In the framework this fact is incorporated by introduction of the abstract class FrequencyRepresentation and its two subclasses ClippedFT and QRegEstimator, where the actual computations are implemented via the method initialization(). The class FrequencyRepresentation serves as a common interface to the quantities in (6). It provides data fields to store various information, including

- the observations Y from which the quantities were computed,
- the frequencies and levels for which the computation was performed, and
- the result of the computation, which is stored in an array values.

Further more, a flag isRankBased indicates whether, prior to the main computations, the observations (Y_t) were transformed to pseudo-observations $(\hat{F}_n(Y_t))$. Performing this extra step will yield $\hat{b}_{n,R}^{\tau}(\omega)$ instead of $\hat{b}_n^{\tau}(\omega)$ or $d_{n,R}^{\tau}(\omega)$ instead of $d_n^{\tau}(\omega)$, respectively. The class BootPos allows for performing a block bootstrap procedure by "shuffling" the observations and repeatedly doing the computations on these bootstrapped observations. Currently only one method, the MovingBlocks bootstrap, is implemented.

Now, turning attention to the class SmoothedPG, recall that the various smoothed periodograms are all defined similarly, in the sense that computing the smoothed periodogram for $\omega_j := 2\pi j/n$, $j=1,\ldots,n-1$ basically means to do a discrete convolution of the sequence of quantile periodograms computed at ω_s with a sequence of appropriately chosen weight functions $W_n(\omega_s)$. Hence, everything needed for the smoothed periodogram is these two ingredients, which is reflected in the framework by two aggregation relationships involving the class SmoothedPG. The first such relationship links SmoothedPG to the QuantilePGs to be smoothed. The second such relationship links SmoothedPG to a class Weight, which provides a common interface to different weight functions. Currently two implementations are included. Employing weights of type KernelWeight, defined by a kernel W and a scale parameter bw (bandwidth), will yield an estimator for the quantile (i. e, Laplace or copula) spectral density. An alternative is to use weights of type SpecDistrWeight, which should yield estimators for the integrated quantile (i. e, Laplace or copula) spectral density.

2.4. Implementation of the quantile-based spectral measures

The classes QuantileSD and IntegrQuantileSD were introduced to the framework to make the quantities (1)–(4) available to the user.

To obtain access to a quantity of the form (1) or (2), an instance of QuantileSD can be created. In this case, a number of R independent copies of a time series of length N are obtained by calling the function ts. The function ts is a parameter to specify the model for which to obtain the model quantity and it handles the simulation process. Then, for each of these time series a QuantilePG object is created and their values are averaged: first across the R independent copies, saving the result to meanPG and an estimation of the standard error to stdError. After that the averages are averaged again for each combination of levels across

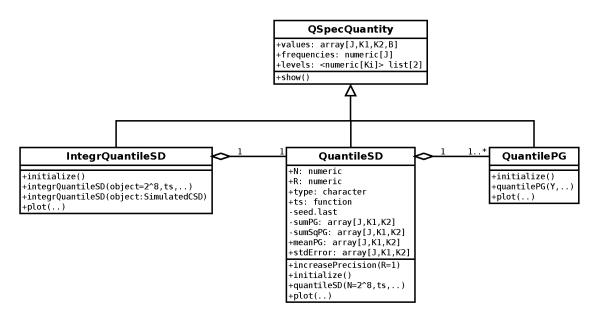


Figure 2: Classes for the numerical computation of (integrated) copula and Laplace spectral densities via simulation

frequencies by smoothing. The result is then made available via the data field values of the superclass. By a call to the method increasePrecision the number of independent copies can be increased at any time to yield a less fluctuating average.

To obtain access to quantities of the form (3) or (4), an instance of IntegrQuantileSD can be created. For the computation an object of type QuantileSD is created and subsequently the integral is approximated via a Riemann sum.

3. Reference implementation: The R-package quantspec

3.1. Overview

The quantspec package (Kley 2014b) is intended to be used both by theoretically oriented statisticians and also by data analysts, who work on a more applied basis. In order to address this broad group of potential users the R system for statistical computing (R Core Team 2012) was chosen as a platform. The R system is particularly well suited for the realization of this project, because it is accessible from many operating systems, without charge, already available to the targeted audience and, in particular, allows to integrate the package's functionality among many other, well developed packages. An important example is that the function rq of the quantreg package (Koenker 2013) could be used.

Both R and the **quantspec** package are available from the comprehensive R archive network (CRAN, http://cran.r-project.org). The package's development is actively continued with the source code available from a GitHub repository (https://github.com/tobiaskley/quantspec). Besides the source code of the releases, which are also available from the CRAN servers, the GitHub repository additionally contains a detailed history of all changes, including comments, that were applied to the source code since April/10/2014, when the GitHub repos-

Constructor	Type of Object	Quantities Computed
clippedFT	ClippedFT	$d_n^q(\omega), d_{n,R}^{\tau}(\omega)$
qRegEstimator	QRegEstimator	$b_n^{ au}(\omega),b_{n,R}^{ au}(\omega)$
${\tt quantilePG}$	QuantilePG	$\hat{L}_n^{ au_1, au_2}(\omega),~\hat{L}_{n.R}^{ au_1, au_2}(\omega),$
		$I_{n}^{q_{1},q_{2}}(\omega),I_{n,R}^{ au_{1}, au_{2}}(\omega)$
${\tt smoothedPG}$	${\tt SmoothedPG}$	$\hat{\mathfrak{f}}_n(au_1, au_2;\omega),\ \hat{\mathfrak{f}}_{n,R}(au_1, au_2;\omega),$
		$\hat{G}_n(q_1,q_2;\omega),\hat{G}_{n,R}(au_1, au_2;\omega)$
quantileSD	QuantileSD	$\mathfrak{f}_{q_1,q_2}(\omega),\mathfrak{f}_{q_{ au_1},q_{ au_2}}(\omega)$
${\tt integrQuantileSD}$	${\tt IntegrQuantileSD}$	$\mathfrak{F}_{q_1,q_2}(\omega),\mathfrak{F}_{q_{ au_1},q_{ au_2}}(\omega)$
kernelWeight	KernelWeight	$W_n(u) = b_n^{-1} \sum_{j=1}^{n} W(b_n^{-1}(u+2\pi j))$
spectrDistrWeight	spectrDistrWeight	$W_n(u) = I\{u \le 0\}$

Table 1: Constructors of the quantspec package that are intended for the end-user.

itory was created. The repository is organized into several branches: the master branch, the develop branch and possibly several topic branches. Since version 1.0-0 the master branch contains the source code of all release candidates and official releases, the develop branch contains the most recent updates and bug fixes that were not yet released. The topic branches contain the source code in which extensions to the package are developed.

To install a package from the source code straight from the repository use the install_github function of the **devtools** package (Wickham and Chang 2013). More precisely, install the **devtools** package, if it's not already installed, and call

R> devtools::install_github("tobiaskley/quantspec", ref="master")

Instead of using "master", another branch (e.g., develop to pull the most recent updates) or a tag that is pointing to one of the releases (e.g., v1.0-0-rc1, to install the 1st release candidate to version 1.0-0) can be used as ref.

Note that the code in the develop branch is merged into the master branch only for a release (candidate) and after being thoroughly tested, so if you're installing from the develop branch you will potentially be using code that has not been fully tested.

Use the option build_vignettes = FALSE if you don't have IATEX installed on your system.

3.2. R code intended for the user and its documentation

The classes of the **quantspec** package, their methods, slots, dependencies and inheritance properties are implemented as conceptually designed [cf. Section 2]. Recall that the design was presented in form of class diagrams, on display in Figures 1 and 2, and that no specific programming language was assumed. All classes that are intended for the end-user possess a constructor method with the same name as the class itself but beginning with a lower case letter. The classes intended for the end-user and their constructors are listed in Table 1.

For a more detailed description of constructors and classes, documentation within the online help system of R is available. After loading the package, which is done by calling

> library(quantspec)

the help file of the package, which provides an overview on the design, can be called by executing

```
> help(quantspec) # alternatively: package?quantspec
```

on the R command line. Note that an index of all available functions can be accessed at the very bottom of the page. If for example more information on the constructor of QRegEstimator and on the class itself is desired, then

```
> help(qRegEstimator)
> help(QRegEstimator) # alternatively: class?QRegEstimator
```

should be invoked. Using this class to determine the frequency representation $b_{n,R}^{\tau}(\omega)$, for $\tau \in \{0.25, 0.5, 0.75\}$ would look as follows. In a toy example, where eight independent random variables $X_0, \ldots, X_7 \sim N(0,1)$ are generated and used to compute $b_{n,R}^{\tau}(\omega)$, call

```
> Y <- rnorm(8)
> bn <- qRegEstimator(Y, levels = c(0.25,0.5,0.75))</pre>
```

By default the computation is done for all Fourier frequencies $\omega = 2\pi j/n \in [0, \pi], n = 8, j = 0, \dots, \lfloor n/2 \rfloor$. The computed information can then be viewed by typing the name of the variable (i. e., bn) to the R console:

> bn

```
QRegEstimator (J=5, K=3, B+1=1)
```

Frequencies: 0 0.7854 1.5708 2.3562 3.1416

Levels : 0.25 0.5 0.75

Values:

```
tau=0.25 tau=0.5 tau=0.75
0 2.000+0.000i 4.000+0.000i 6.000+0.000i
0.785 0.439+0.354i 0.854-0.646i 0.939-0.561i
1.571 -1.750-0.250i -0.250+0.750i -0.750+0.250i
2.356 -0.732+0.354i -0.914-0.086i -1.621+0.379i
3.142 0.500+0.000i 1.000+0.000i 0.500+0.000i
```

Methods other than the constructor are implemented as generic functions. To invoke the method f of an object obj the call therefore is f(obj). In particular all attributes mentioned in the class diagram can be accessed via getter methods. There are no setter methods, because all attributes are completely handled by internal functions. For an example, to retrieve the attributes frequencies and parallel of the object bn, execute the following lines on the R shell

```
> getFrequencies(bn)
```

```
[1] 0.0000000 0.7853982 1.5707963 2.3561945 3.1415927
```

```
> getParallel(bn)
```

[1] FALSE

To invoke a method f with parameters p1,...,pk of an object obj the call is f(obj,p1,...,pk). An example is to invoke the accessor function getValues, which is equipped with parameters to get the values associated with certain frequencies or levels. An exemplary call looks like this:

```
> getValues(bn, levels = c(0.25,0.5))
```

, , 1

Note that the result is returned as an array of dimension c(J,K,B+1), where in the present case B=0 bootstrap replications were performed. For a detailed description on how to use the function getValues in the above mentioned case, access the online help via the command

```
> help("getValues-FreqRep")
```

Note the format method_name-class_name to access the help page of a method and that the attribute values is part of the abstract class FreqRep [cf. Figure 2].

A graphical representation of the data can easily be created by applying the plot command. For example, to compute and plot the frequency representations $d_{32,R}^{\tau}(\omega)$, from 32 simulated, standard normally distributed random variables execute the following lines on the R shell:

```
> dn <- clippedFT(rnorm(32), levels = seq(0.05,0.95,0.05))
> plot(dn, frequencies = 2*pi*(0:64)/32, levels = c(0.25,0.5))
```

The above script will yield the diagrams that are on display in Figure 3. Note that the $d_{32,R}^{\tau}(\omega)$ were determined for $\tau \in \{0.05, 0.1, \dots, 0.9, 0.95\}$ and, by the default setting, for all Fourier frequencies from $[0, \pi]$. The plot, however, was parameterized to show only $\tau \in \{0.25, 0.5\}$, but all Fourier frequencies from $[0, 4\pi]$; by default all available levels and frequencies would be used. In this example two of the 19 frequencies were selected to yield a plot of a size that is appropriate to fit onto the page. Further more, the plot was parameterized to show $d_{n,R}(\omega)$ for all Fourier frequencies from $[0, 4\pi]$ to illustrate characteristic redundancies

13

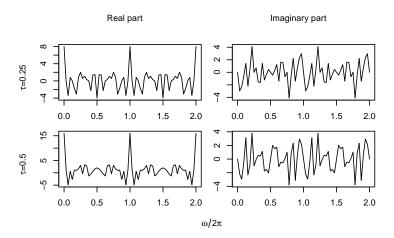


Figure 3: Plot of the FrequencyRepresentation object bn

in the frequency representation objects, and to point out that the default values are always sufficient. The two relations

$$d_{n,R}^{\tau}(\omega) = \overline{d_{n,R}^{\tau}(2\pi - \omega)}, \quad d_{n,R}^{\tau}(\omega) = d_{n,R}^{\tau}(\omega + 2\pi j),$$

hold for any $\omega \in \mathbb{R}$ and $j \in \mathbb{Z}$, $d_{n,R}^{\tau}(\omega)$. Therefore, without additional calculations, the plot of $d_{n,R}^{\tau}(\omega)$ can be determined for any $\omega \in 2\pi j/n$, $j \in \mathbb{Z}$, as long as $d_{n,R}^{\tau}(\omega)$ is known for $\omega \in 2\pi j/n$, $j = 0, \ldots, \lfloor n/2 \rfloor$, which is what is determined by the default setting. Note that all of this happens transparently for the user, as the method **getValues** takes care of it. Another fact that one can presume by inspecting Figure 3 is that $d_{n,R}^{\tau}(\omega)$ appears to be uncorrelated and centered (for $\omega \neq 0 \mod 2\pi$).

3.3. Additional elements of the package

The quantspec package includes three demos that can be accessed via

- > demo(sp500)
- > demo(wheatprices)
- > demo("qar-simulation")

Several examples explaining on how to use the various functionality can be found in the online help files or the folder examples in the directory where the package is installed. The package comes with two data sets sp500 and wheatprices that are used in the demos and in the examples.

A package vignette amends the online help files. It contains the text of this paper.

Unit tests covering all main functions were implemented using the **testthat** framework (Wickham 2011).

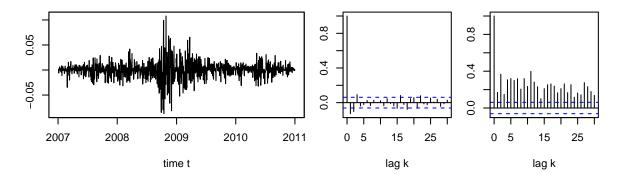


Figure 4: Returns (Y_t) of the S&P 500 returns example data (left), autocovariances $Cov(Y_{t+k}, Y_t)$ of the returns (middle), and autocovariances $Cov(Y_{t+k}^2, Y_t^2)$ of the squared returns (right)

4. Two worked examples

4.1. Analysis of the S&P 500 stock index, 2007-2010

In this section the use of the **quantspec** package from the perspective of a data analysts is explained. To this end an analysis of the returns of the S&P 500 stock index is performed. Note that a similar analysis and the data set used are available in the package. Calling demo("sp500") will start the computations and by sp500 the data set can be referenced to do additional analysis.

For the example the years 2007 through to 2010 were selected to have a time series that, at least to some degree, can be considered stationary. Aside from this more technical consideration, employing the new statistical toolbox will reveal interesting features in the returns collected in the financial crisis that completely escape the analysis with the traditional tools blindly applied.

For a start, use the following R script to plot the data, the autocovariances of the returns and the autocovariances of the squared returns.

The three plots are displayed in Figure 4. Inspecting them, it is important to observe that the returns themselves appear to be almost uncorrelated. Therefore, not much insight into the serial dependency structure of the data can be expected from traditional spectral analysis. The squared returns on the other hand are significantly correlated. This observation, typically taken as an argument to fit an ARCH or GARCH model, clearly proves that serial dependency exists. In what follows the copula spectral density will be estimated from the data, using quantile periodograms and smoothing them. It will be seen that using the **quantspec** package this can be done with only a few lines of code necessary.

First, take a look at the CR periodogram $I_{n,R}^{\tau_1,\tau_2}(\omega)$. In the **quantspec** package it is represented as a QuantilePG object and can be computed calling the constructor function quantilePG with the parameter type = "clipped". To do the calculation for $\tau_1,\tau_2\in\{0.05,0.5,0.95\}$, all Fourier frequencies ω and with 250 bootstrap replications determined from a moving blocks bootstrap with block length $\ell=32$, it suffices to execute the first command of the following script:

```
> CR <- quantilePG(sp500, levels.1 = c(0.05,0.5,0.95),
+ type = "clipped", type.boot = "mbb", B = 250, 1 = 32)
> freq <- getFrequencies(CR)
> plot(CR, levels = c(0.05,0.5,0.95),
+ frequencies = freq[freq > 0 & freq <= pi],
+ ylab = expression({I[list(n,R)]^{list(tau[1],tau[2])}}(omega)))</pre>
```

Using the second command it is possible to learn for which frequencies the values of the CR periodogram are available. As pointed out in the previous paragraph it was computed for all Fourier frequencies from the interval $[0,2\pi)$, which is the default setting for quantilePG and smoothedPG. With the third command the graphical representation of the CR periodogram, which can be seen in Figure 5, is plotted. The plot seen here is a typical plot of any QSpecQuantity: in a configuration with K levels the plot has the form of a $K \times K$ matrix, where the subplots on and below the diagonal display the real part of the CR periodogram $I_{n,R}^{\tau_1,\tau_2}(\cdot)$, with the levels τ_1 and τ_2 denoted on the left and bottom margins of the plot. Above the diagonal the imaginary parts are shown.

To observe the larger values in the neighborhood of $\omega = 0$ and in the extreme quantile levels more closely a plot showing the CR periodogram only for frequencies $\omega \in [0, \pi/5]$ can be generated using the following script:

```
> plot(CR, levels = c(0.05,0.5,0.95),
+ frequencies = freq[freq > 0 & freq <= pi/5],
+ ylab = expression({I[list(n,R)]^{list(tau[1],tau[2])}}(omega)))</pre>
```

The plot is shown in Figure 6.

In the next step the computed quantile periodogram CR can be used as the basis to determine a smoothed CR periodogram sCR. In the form of a SmoothedPG object it can be generated by the constructor smoothedPG of that class. Besides the QuantilePG object CR, a KernelWeight object is required, which is easily generated using the constructor kernelWeight. As parameters the constructor kernelWeight requires a kernel W and a bandwidth bw. The quantspec package comes with several kernels already implemented. The Epanechnikov kernel for example can be referred to by the name W1. For a complete list of the available kernels call

```
> help(kernels)
```

To compute the smoothed CR periodogram from CR using the Epanechnikov kernel and bandwidth bw = 0.07 the first of the following two commands need to be executed.

```
> sPG <- smoothedPG(CR, weight=kernelWeight(W=W1, bw=0.07))
> plot(sPG, levels = c(0.05,0.5,0.95), type.scaling = "individual",
+ frequencies = freq[freq > 0 & freq <= pi], ptw.CIs = 0.1,
+ ylab = expression(hat(G)[list(n,R)](list(tau[1],tau[2],omega))))</pre>
```

Of course, the second line initiates plotting the smoothed CR periodogram, which is on display in Figure 7. Note that the option type.scaling can be set to yield a plot with certain subplots possessing the same scale. In Figure 7 pointwise confidence intervals are shown. By default these are determined using a normal approximation to the distribution of the estimator as is suggested by the limit theorem in Kley et al. (2014). An alternative is to use the quantiles of estimates computed from the block bootstrap replicates. These pointwise confidence intervals can be plotted using the option type.CIs = "boot.full", as is shown in the following script:

```
> plot(sPG, levels = c(0.05,0.5,0.95), type.scaling = "real-imaginary",
+ ptw.CIs = 0.1, type.CIs = "boot.full",
+ frequencies = freq[freq > 0 & freq <= pi],
+ ylab = expression(hat(G)[list(n,R)](list(tau[1],tau[2],omega))))</pre>
```

For illustrative purposes a different type of scaling was used for the second plot. A complete description of the options available is available in the online help, which can be accessed by calling

```
> help("plot-SmoothedPG")
```

Inspecting the plots in Figures 7 and 8 reveals that serial dependency in the events $\{Y_t \leq q_{0.05}\}$ and $\{Y_t \leq q_{0.95}\}$ is present in the data. This concludes the introduction of the **quantspec** package for data analysts and we can continue with the presentation of how it can also make the work of a probability theorist easier.

Tobias Kley 17

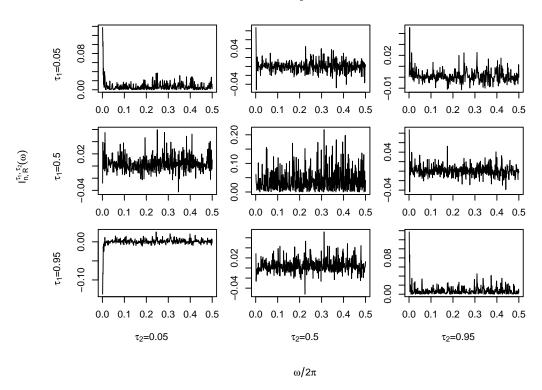


Figure 5: Plot of the QuantilePG object CR, computed from the sp500 time series; $\omega \in (0,\pi]$

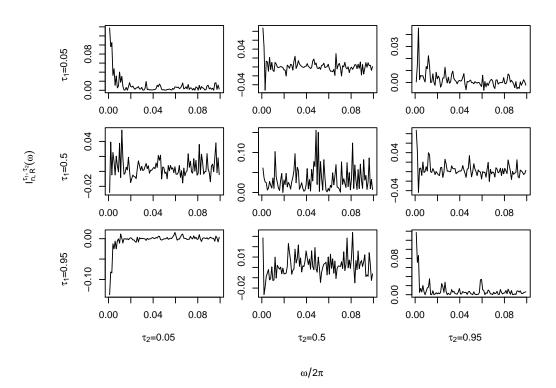


Figure 6: Plot of the QuantilePG object CR, computed from the sp500 time series; $\omega \in (0,\pi/5]$

.

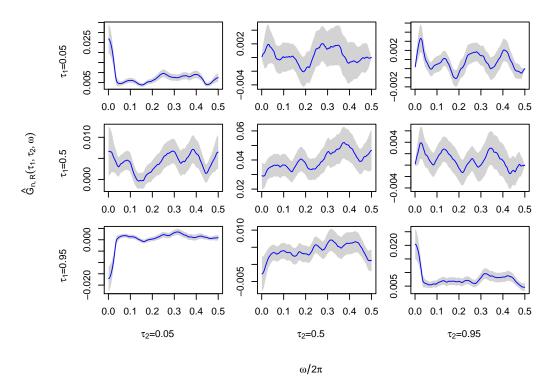


Figure 7: Plot of the SmoothedPG object sCR, computed from the sp500 time series; type.scaling = "individual", ptw.CIs = 0.1

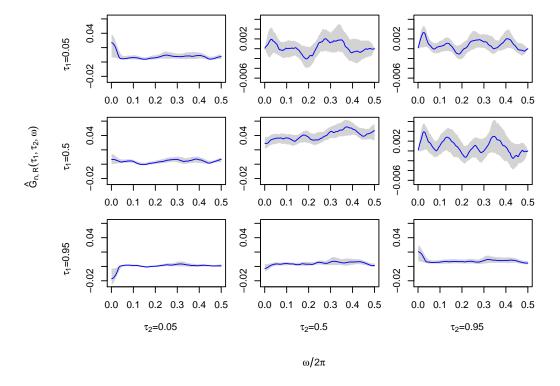


Figure 8: Plot of the SmoothedPG object sCR, computed from the sp500 time series; type.scaling = "real-imaginary", ptw.CIs = 0.1, type.CIs = "boot.full"

4.2. A simulation study – analysing a quantile autoregressive process

In this section using the **quantspec** package from the perspective of a probability theorist is explained. The aim is twofold. On the one hand, further insight into a stochastic process shall be gained. Any process for which a function to simulate finite stretches of is available can be studied. On the other hand, the finite sample performance of the new spectral methods are to be evaluated. Note that the example discussed in this section and the functions to simulate QAR(1) processes are available inside the package, by calling demo("qar-simulation") and by referring to the function ts1, which implements the QAR(1) process that was discussed in Dette $et\ al.\ (2013)$ and Kley $et\ al.\ (2014)$. Recall that a QAR(1) process is a sequence (X_t) of random variables that fulfills

$$X_t = \theta_1(U_t)X_{t-1} + \theta_0(U_t),$$

where U_t is independent white noise with $U_t \sim \mathcal{U}[0,1]$ (Koenker and Xiao 2006). The function ts1 implements the model, where $\theta_1(u) = 1.9(u - 0.5)$, $u \in [0,1]$ and $\theta_0 = \Phi^{-1}$, which was discussed in Dette *et al.* (2013) and Kley *et al.* (2014). A complete list of models included in the package can be seen in the online documentation of the package by calling

```
> help("ts-models")
```

The following, two-line script can be used to generate the graphical representation of the copula spectral density that is on display in Figure 9

```
> csd < quantileSD(N=2^9, seed.init = 2581, type = "copula",
+ ts = ts1, levels.1 = c(0.25, 0.5, 0.75), R = 100, quiet=TRUE)
> plot(csd, ylab = expression(f[list(q[tau[1]],q[tau[2]])](omega)))
```

When analysing a time series model the recommended practice is to compute the quantile spectral density once with high precision, store it to the hard drive, and load it later whenever it is needed. The following two lines of code can be used to do this:

```
> csd < quantileSD(N=2^12, seed.init = 2581, type = "copula", 
+ ts = ts1, levels.1 = c(0.25, 0.5, 0.75), R = 50000)
> save(csd, file="csd-qar1.rdata")
```

With the first configuration $(N=2^9 \text{ and } R=100)$ the computation time was only around three seconds. To compute the second csd object (with $N=2^{12}$ and R=50000) the same machine needed roughly 2.5 hours. Storing the object in a file takes about 1MB of hard disk space. Not only values and stdErrors are stored within the QuantileSD object; also the final state of the pseudo random number generator is stored and the method increasePrecision can be used to add more simulation runs at any time to yield a better approximation to the true quantile spectrum. More information on this method can be found in the online help, which is accessible via

```
> help("increasePrecision-QuantileSD")
```

Once the computation is finished the diagram on display in Figure 10 can be created using the following two lines of code:

```
> load("csd-qar1.rdata")
> plot(csd, frequencies = 2*pi*(1:2^8)/2^9,
+ ylab = expression(f[list(q[tau[1]],q[tau[2]])](omega)))
```

The parameter frequencies was used when plotting the copula spectral density to create a plot that can be compared to the one in Figure 9. Note that by default the plot would have been created using all available frequencies which yields a grid of 8 times as many points on the x-axis $(N=2^{12} \text{ vs. } N=2^9)$. Now, to get a first idea of how well the estimator performs plot the smoothed CR periodogram computed from one simulated QAR(1) time series of length 512:

```
> sCR <- smoothedPG(ts1(512), levels.1 = c(0.25,0.5,0.75),
+ weight=kernelWeight(W=W1, bw=0.1))
> plot(sCR, qsd = csd,
+ ylab = bquote(paste(hat(G)[list(n,R)](list(tau[1],tau[2],omega)),
+ " and ", f[list(q[tau[1]],q[tau[2]])](omega))))
```

The generated plot is on display in Figure 11. It is worth pointing out that in this example the estimator performs already quite well. Note that a different version of the constructor smoothedPG was used here than in Section 4.1. When computing a smoothed quantile periodogram straight from a time series, the syntax is the same as for quantilePG, but with the additional parameter weight.

Finally, for the simulation study, a number of R=5000 independent QAR(1) time series are generated. Before the actual simulations, some variables that determine what is to be simulated are defined:

```
> set.seed(2581)
> ts <- ts1
> N <- 128
> R <- 5000
> freq <- 2*pi*(1:16)/32
> levels <- c(0.25, 0.5, 0.75)
> J <- length(freq)
> K <- length(levels)
> sims <- array(0, dim=c(4,R,J,K,K))
> weight <- kernelWeight(W=W1, bw=0.3)</pre>
```

Setting the seed in the very beginning allows for reproducible results. Recall that ts1 is a function to simulate from the QAR(1) model to be studied. N is the length of the time series and also the number of Fourier frequencies for which the quantile periodograms will be computed. By the parameter freq a subset of these Fourier frequencies is specified to be stored; a subset is used to save storage space. The estimates at these frequencies freq and at the specified levels are then stored to the array sims. In this example, the smoothed periodograms are computed using the Epanechnikov kernel and the (rather large) bandwidth of $b_n = 0.3$.

Tobias Kley 21

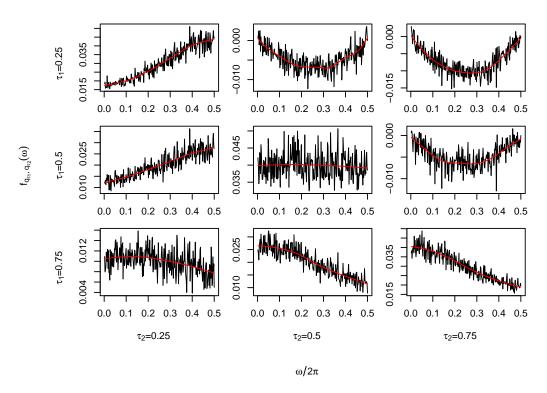


Figure 9: Plot of the copula spectral density $\mathfrak{f}_{q_{\tau_1},q_{\tau_2}}(\omega)$ of the QAR(1) model; $\tau_1,\tau_2\in\{0.25,0.5,0.75\}$, and $\omega\in[0,\pi];\,N=2^9$ and R=100.

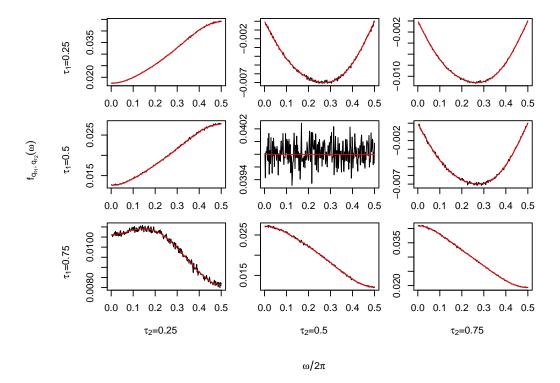


Figure 10: Plot of the copula spectral density $\mathfrak{f}_{q_{\tau_1},q_{\tau_2}}(\omega)$ of the QAR(1) model; $\tau_1,\tau_2\in\{0.25,0.5,0.75\}$, and $\omega\in[0,\pi]$; $N=2^{12}$ and R=50000.

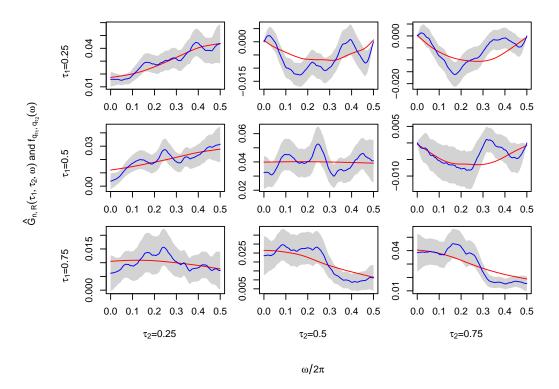


Figure 11: Plot of a smoothed CR periodogram, computed from one realization of a QAR(1) time series; n = 512, Epanechnikov kernel with $b_n = 0.1$.

For the actual simulation the following for loop can be used:

Note that the flexible accessor method getValues is used to access the relevant subset of values for the frequencies specified (i.e., freq). Once the array sims is available, many interesting properties of the estimator can be analyzed. Examples include the bias, variance, etc. Here, using the function getValues again, the true copula spectral density is copied to an array trueV. Using the arrays sims and trueV the root integrated mean squared errors are computed as follows:

Tobias Kley

```
> trueV <- getValues(csd, frequencies=freq)</pre>
> SqDev <- array(apply(sims, c(1,2),
          function(x) {abs(x-trueV)^2}), dim=c(J,K,K,4,R))
> rimse <- sqrt(apply(SqDev, c(2,3,4), mean))</pre>
R> rimse
, , 1
           [,1]
                       [,2]
                                   [,3]
[1,] 0.03292733 0.03543752 0.02879294
[2,] 0.03543752 0.04113916 0.03427386
[3,] 0.02879294 0.03427386 0.03014753
, , 2
           [,1]
                       [,2]
                                   [,3]
[1,] 0.02688713 0.03414821 0.03113987
[2,] 0.03414821 0.03447605 0.03341930
[3,] 0.03113987 0.03341930 0.02526853
, , 3
            [,1]
                         [,2]
[1,] 0.004338658 0.005889695 0.004472232
[2,] 0.005889695 0.006794010 0.005428915
[3,] 0.004472232 0.005428915 0.004917286
            [,1]
                         [,2]
                                      [,3]
[1,] 0.005133099 0.011058309 0.015858590
[2,] 0.011058309 0.006179652 0.010963587
[3,] 0.015858590 0.010963587 0.004797474
```

These numbers could now be inspected to, for example, observe that the smoothed quantile periodogram possess smaller root integrated mean squared errors than the quantile periodograms (without smoothing). Further discussion of the numbers is omitted, because the crux of this chapter was to explain how to perform the simulation study, not to actually do it.

5. Roadmap to future developments and concluding remarks

As the new methodology evolves additional features will be added to the **quantspec** package. For each new feature an entry to the issue tracker available on the GitHub will be made. Then the new feature will be implemented on a topic branch of the repository. For example, a procedure for data-driven selection of the bandwidth is currently being developed.

Other, more complex extensions to the software include the implementation of function to perform quantile spectral analysis for locally stationary processes, the computation and smoothing of higher order quantile periodograms for the estimation of quantile polyspectra. Procedures for graphical representations of these object, possibly animated ones, will amend these planned parts of the package. An overview on the planned extensions will be made available in the issue tracker on GitHub.

Summing up, it can be said that the **quantspec** package provides a comprehensive and conclusive toolbox to perform quantile-based spectral analysis. Due to the great interest in and active development of the statistical procedures that are quantile-based spectral analysis it was deliberately designed in an object-oriented and extensible design. Thus it is well prepared for the many extensions that are sure to come in the near future. The source code is open and extensive documentation of the system freely available. Comments on and contribution to the project is, of course, very much welcome.

Acknowledgments

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25

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