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Forecasting probability density functions in Hilbert spaces

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Resumo

A Análise de Dados Funcionais (Functional Data Analysis – FDA) tem emergido como um campo em rápida evolução, estendendo os métodos estatísticos clássicos para dados representados por funções. Nesse contexto, a análise de séries temporais também pode ser generalizada ao tratar cada observação como uma função, em vez de um escalar ou vetor. Este trabalho foca na previsão de uma classe específica de objetos funcionais: as funções densidade de probabilidade (FDPs). Um dos principais desafios nesse cenário surge do fato de que PDFs não formam um espaço vetorial, mas residem em um subconjunto convexo, tornando as técnicas padrão de séries temporais funcionais uma tarefa complexa. Para contornar isso, propõe-se uma abordagem de transformação linear que mapeia FDPs em um espaço de Hilbert, permitindo a aplicação de técnicas consolidadas de séries temporais funcionais. A eficácia dessa abordagem é ilustrada por meio de uma aplicação em dados financeiros de alta frequência.

Palavras-chaves: Análise de dados funcionais. Séries temporais funcionais. Funções de densidade de probabilidade. Projeção. Expansão de Karhunen-Loève.

Abstract

Functional Data Analysis (FDA) has emerged as a rapidly evolving field, extending classical statistical methods to data represented by functions. In this context, time-dependent analysis can also be generalized by treating each observation as a function rather than a scalar or vector, giving rise to functional time series. This work focuses on forecasting a specific class of functional objects: probability density functions (PDFs). A key challenge in this setting arises from the fact that PDFs do not form a vector space, but instead reside in a convex subset, rendering standard functional time series techniques a tricky endeavor. To address this, we propose a transformation approach that maps PDFs into a Hilbert space, enabling the application of established functional time series tools. The effectiveness of this method will be illustrated through an application to high-frequency financial data, with results highlighting its potential compared to other state-of-the-art tools for accurate and interpretable forecasting.

Keywords: Functional data analysis. Functional time series. Probability density functions. Forecasting. Karhunen-Loève expansion.

Sumário

1 Introduction

1.1 Context

High-frequency trading (HFT) represents a significant evolution in modern financial markets, characterized by the execution of large volumes of trades at extremely high speeds. In such an environment, traditional assumptions of financial econometrics—such as normally distributed returns or independent and identically distributed (i.i.d.) increments—frequently break down. As a result, the specification of the probability density function (PDF) governing price changes or returns becomes a foundational aspect of modeling, forecasting, and executing trades in HFT systems.

PDF specification allows practitioners to move beyond point forecasts and assess the full range of possible future price realizations. This is particularly important in high-frequency contexts, where price changes are often small but frequent, and the tail behavior of the distribution can have outsized impacts on profitability and risk. Accurate modeling of PDFs aids in several key HFT tasks, including order placement, market making, liquidity provision, and statistical arbitrage.

Empirical studies have shown that the distributions of high-frequency returns exhibit heavy tails, volatility clustering, and non-Gaussianity, especially over very short horizons (CONT, 2001). Mischaracterizing these features can result in substantial model risk, leading to incorrect probability estimates and suboptimal execution. For instance, assuming normality in return distributions can underestimate the likelihood of large price swings, increasing exposure to adverse selection or sudden liquidity shocks.

Various models have been proposed to better capture the observed dynamics of high-frequency data. Nonparametric and semiparametric methods, such as kernel density estimation and mixture models, offer flexibility in modeling the empirical PDF without overly restrictive distributional assumptions (FAN; YAO, 2003). On the parametric side, models based on generalized hyperbolic distributi-

ons (PRAUSE, 1999), α-stable distributions (NOLAN, 2003), and autoregressive conditional duration (ACD) models (ENGLE; RUSSELL, 1998) have been shown to provide better fits to high-frequency financial time series.

In practical HFT systems, the real-time estimation of these PDFs is often embedded in algorithmic decision engines. For example, limit order placement algorithms rely on an accurate forecast of the short-term price movement distribution to maximize expected fill rates while minimizing adverse selection risk (CARTEA; JAIMUNGAL; PENALVA, 2015). Similarly, market-making strategies use estimates of the conditional PDF to dynamically adjust bid-ask spreads based on the predicted volatility and direction of price changes.

Thus, the specification of the probability density function is not merely a statistical exercise, but a key driver of performance in high-frequency trading. It directly informs the risk-reward trade-offs of algorithmic strategies and serves as a bridge between quantitative modeling and microstructural market dynamics.

1.2 A glimpse into Functional Data Analysis

An alternative to this analysis is to interpret PDFs as a sequence of random functions, which would allow a researcher to forecast its value for a specific time horizon. This is where Functional Data Analysis (FDA), an extension from Multivariate Data Analysis (MDA), comes into play. First off, we may recall that Multivariate Data Analysis encompasses a collection of techniques designed to analyze data that arises from more than one variable. Unlike univariate or bivariate methods, MDA seeks to explore the structure and relationships that exist in datasets with multiple interdependent measurements, enabling a more comprehensive understanding of complex phenomena that are obserserved in fields such as biology, economics and finance. Techniques such as Principal Component Analysis (PEARSON, 1901), Factor Analysis, Cluster Analysis and Canonical Correlation (HOTELLING, 1936) enable one to reduce dimensionality, detect latent structures, and model the joint distribution of variables.

Functional Data Analysis, by its turn, is a statistical framework for analyzing data that can be represented by functions, curves, or trajectories over a continuum such as time, space, or frequency. Unlike traditional multivariate analysis, which handles data as finite-dimensional vectors, FDA treats each observation as a function, often lying in an infinite-dimensional Hilbert space. This perspective is especially useful for studying processes that evolve continuously, such as temperature records, electroencephalogram (EEG) signals or financial intraday returns.

The foundational developments in FDA began with the pioneering work of Ramsay (1982), who introduced spline smoothing techniques for curve estimation. In their influential texts, Ramsay e Silverman (2005) and Ferraty (2006) developed a unified theory that encompasses functional principal component analysis (FPCA), functional regression, and clustering of functional observations.

One of the earliest practical applications of FDA was in growth curve analysis, where children's height measurements taken at different ages were analyzed as smooth trajectories (RAMSAY; DALZELL, 1991). Since then, FDA has seen widespread use in meteorology, biomechanics, and econometrics. Some modern extensions now integrate FDA with machine learning and time series models.

The core challenge in FDA lies in adapting classical statistical techniques to infinite-dimensional spaces. This requires tools from functional analysis, such as basis function expansions (e.g., splines, Fourier, wavelets), and the use of inner product structures for defining distances and covariances between functions. These methods enable dimension reduction (via FPCA), classification, hypothesis testing, and regression in the functional domain.

Further, if we consider each of the curves to be time-dependent, we obtain a *functional time series* (FTS) object, which is simply a sequence of random functions indexed by time. Each observation in the series is a function, typically lying in an infinite-dimensional function space. In this case, let $\mathcal{H}$ be the separable Hilbert space $L^2(\mathcal{I})$, the space of square-integrable functions on a compact interval $\mathcal{I} \subseteq \mathbb{R}$, equipped with an inner product. A foundational treatment of linear models for functional data was provided by Bosq (2000), who developed autoregressive models

in a Hilbert space setting, laying the groundwork for many later developments in the field. His approach enabled the extension of classical time series concepts like stationarity and autocorrelation to the infinite-dimensional setting. This leads to a possibility of forecasting objects like PDFs, but some caveats related to the nature of this type of data must be considered.

1.3 Compositional Data Analysis

Compositional data (CoDa) are multivariate observations conveying relative information, typically represented as vectors with strictly positive components summing to a constant like 1 or 100% (AITCHISON, 1982). Such data arise naturally in diverse disciplines, but are specially related to the context of this research since we are dealing with probability measures.

Classical multivariate statistical techniques often fail to appropriately handle the specific properties of compositional data due to the constant-sum constraint and the inherent relative scale of the data. As a consequence, applying standard techniques directly to raw compositional data can lead to misleading results (PAWLOWSKY-GLAHN; EGOZCUE; TOLOSANA-DELGADO, 2015). Aitchison's work (AITCHISON, 1986) laid the foundation for the modern statistical treatment this problem. He introduced the use of log-ratio transformations, such as the centered log-ratio (clr), additive log-ratio (alr), and isometric log-ratio (ilr) transformations, to enable the application of standard statistical tools in an appropriate transformed space. These transformations map the data from the simplex (the sample space of compositions) to real Euclidean space, facilitating analysis while preserving the essential relative information.

The simplex, denoted as $\mathcal{S}^D = \left\{\mathbf{x} = (x_1, \ldots, x_D) \in \mathbb{R}^D_{>0} : \sum_{i=1}^D x_i = \kappa\right\}$, where κ is a positive constant (typically 1 or 100), serves as the sample space for compositional data (EGOZCUE et al., 2003). A key aspect of CoDa is the use of the Aitchison geometry on the simplex, which redefines operations such as

perturbation (compositionally meaningful addition) and powering (compositionally meaningful scalar multiplication).

An important and growing extension of CoDa is its adaptation to probability density functions (PDFs), which share a key compositional property: they are non-negative and integrate to one. This extension is formally developed within the framework of *Bayes spaces*, where PDFs are treated as infinite-dimensional compositional objects (EGOZCUE; DÍAZ-BARRERO; PAWLOWSKY-GLAHN, 2006). The centered log-ratio (clr) transformation is generalized to functions, allowing PDFs to be analyzed in a Hilbert space endowed with the Aitchison geometry.

2 Goal

The main goal of this work is to assess the viability of forecasting functional time series that inherently carry relative information. Specifically, the functional observations are probability density functions, which are subject to the following constraints:

Proposition 1. *Let $f_X(x)$ denote the density function of a continuous random variable X, defined on the probability space $(\Omega, \mathbb{F}, \mathbb{P})$. Then $f_X(x)$ satisfies*

1. *$f_X(x) \geq 0$, for all x in $\mathbb{R}$*
2. *$\int_{-\infty}^{\infty} f(w)dw = 1$*

The precise objectives are to

1. Perform data analysis of the time series subject to the study;
2. Evaluate time series decomposition, i.e., its dimensionality;
3. Find the best time series model fitting to the principal component scores;
4. Obtain a set of forecast values for the probability density functions;
5. Evaluate the performance of the predictions within an application.

3 Literature Review

4 Framework

First, we might define some useful concepts that are present in most works about functional time series.

Definition 1 (Inner product)**.** *Let V be a vector space over a field $\mathbb{K}$, where $\mathbb{K}$ is either $\mathbb{R}$ or $\mathbb{C}$. An inner product on V is a function*

$$\langle \cdot, \cdot \rangle : V \times V \to \mathbb{K}$$

that satisfies the following properties for all $u, v, w \in V$ and all scalars $\alpha \in \mathbb{K}$:

1. *Conjugate symmetry: $\langle u, v \rangle = \overline{\langle v, u \rangle}$*
2. *Linearity in the first argument: $\langle \alpha u + w, v \rangle = \alpha \langle u, v \rangle + \langle w, v \rangle$*
3. *Positive-definiteness: $\langle v, v \rangle \geq 0$, with equality if and only if $v = 0$*

Definition 2 (Hilbert Space)**.** *A Hilbert space is a vector space $\mathcal{H}$ over $\mathbb{K}$ equipped with an inner product $\langle \cdot, \cdot \rangle$, such that $\mathcal{H}$ is complete with respect to the norm induced by the inner product*

$$\|v\| = \sqrt{\langle v, v \rangle},$$

that is, every Cauchy sequence[1] *in $\mathcal{H}$ converges to a limit in $\mathcal{H}$.*

Definition 3 (Functional time series)**.** *Let $\mathcal{H}$ be a separable Hilbert space taken to be $\mathcal{H} = L^2(\mathcal{I})$, that is, the space of square-integrable functions on a compact interval $\mathcal{I} \subset \mathbb{R}$, equipped with the inner product*

$$\langle f, g \rangle = \int_{\mathcal{I}} f(t) g(t)\, dt, \tag{1}$$

and the associated norm $\|f\| = \sqrt{\langle f, f \rangle}$. A functional time series *is a sequence of $\mathcal{H}$-valued random variables $\{X_t\}_{t \in \mathbb{Z}}$, where each X_t is a random element of $\mathcal{H}$, i.e., $X_t : \Omega \to \mathcal{H}, t \in \mathbb{Z}$.*

[1] A sequence $\{v_n\}$ in a metric space $\mathcal{H}$ is called a *Cauchy sequence* if for every $\epsilon > 0$, there exists an integer N such that for all $m, n \geq N$, we have $\|v_n - v_m\| < \epsilon$.

Definition 4 (Karhunen–Loève Expansion)**.** *Let $X(t)$, $t \in \mathcal{I} \subseteq \mathbb{R}$, be a square-integrable stochastic process with mean function $\mu(t) = \mathbb{E}[X(t)]$ and covariance function*

$$C(s,t) = Cov(X(s), X(t)) = \mathbb{E}[(X(s) - \mu(s))(X(t) - \mu(t))]. \tag{2}$$

Then, if $C(s,t)$ is continuous and positive semi-definite, the Karhunen–Loève Expansion of $X(t)$ is given by

$$X(t) = \mu(t) + \sum_{k=1}^{\infty} \xi_k \phi_k(t), \tag{3}$$

where $\{\phi_k(t)\}_{k=1}^{\infty}$ are the orthonormal eigenfunctions of the covariance operator associated with $C(s,t)$; $\{\xi_k\}_{k=1}^{\infty}$ are uncorrelated random variables with zero mean and variances equal to the corresponding eigenvalues λ_k, and $\{\xi_{tk}, k \geq 1\}$ is a ranked set such that $Var(\xi_{tk}) = \lambda_k$ is monotonically decreasing as k increases; and $\mathbb{E}[\xi_k \xi_j] = \lambda_k \delta_{kj}$, with δ_{kj} being the Kronecker delta.

If we consider an observed functional time series object Y_t, we define

$$Y_t(u) = X_t(u) + \varepsilon_t(u), \quad u \in \mathcal{T}, \quad t = 1, \ldots, n, \tag{4}$$

where the noise term $\varepsilon_t(u)$ is originated from experimental error and numerical rounding in discrete data treatment.

Now, we may ask ourselves how to deal with this type of data. In Bosq (2000), we can find a *functional autoregressive* (FAR) approach for time series forecasting, and this has long been the main method used in research because of the lack of other techniques. Nevertheless, the work of Aue, Norinho e Hörmann (2015) proposes a simplification of functional time series prediction by reducing it to a multivariate forecasting problem, thereby allowing the use of well-established tools, in contrast with the methodology of the FAR(p) model. The proposed algorithm consists of three steps: first, a number d of principal components is selected to retain $(\alpha \cdot 100)\%$ of the variance of the original data; then, given a forecast horizon h, a VAR(p) model is fitted to the principal components, and an h-step-ahead forecast is computed; finally, the multivariate forecasts are transformed back to

the original functional space via a truncated Karhunen–Loève representation. It is also shown that the one-step-ahead forecast from a VAR(1) model in the second step is asymptotically equivalent to that of a FAR(1) model, which simplifies the forecasting task. Another important contribution of the paper is the proposal of a fully automatic and joint procedure for selecting the model order p and the number of components d through the minimization of a functional final prediction error (fFPE) criterion given by

$$fFPE(p,d) = \frac{n+pd}{n-pd}\mathrm{tr}(\hat{\Sigma}_Z) + \sum_{l>d}\hat{\lambda}_l, \tag{5}$$

which makes the proposed methodology entirely data-driven. The possibility of including exogenous variables in the model is also supported without major theoretical complications. Finally, simulation studies and applications to real data compare the performance of the new methodology with that of Hyndman e Ullah (2007), which carries out forecasting by treating the principal component scores as univariate time series, and Bosq (2000), using the autoregressive order selection criterion proposed by Kokoszka e Reimherr (2013). In both settings, the new method outperformed the alternatives. We can therefore conclude that this is a useful solution for the problem at hand.

Bathia, Yao e Ziegelmann (2010) propose a way to identify the dimensionality of these objects while modeling the serial dependence of the time series. Under stationarity assumptions, equation 3 tells $X_t(\cdot)$ is d-dimensional if $\lambda_d \neq 0$ and $\lambda_{d+1} = 0$, where $d \geq 1$ is a finite integer. What these authors propose is precisely to determine d and $\mathcal{M} = \mathbf{span}\{\phi_1, ..., \phi_d\}$. For a given lag $k \geq 1$, let the lag-k autocovariance operator be

$$M_k(u,v) = \mathrm{Cov}(X_t(u), X_{t+k}(v)). \tag{6}$$

Since $\varepsilon_t(\cdot)$ is assumed to be white noise and independent across t, $M_k(u,v)$ can be estimated directly from $Y_t(\cdot)$ via:

$$\widehat{M}_k(u,v) = \frac{1}{n-p}\sum_{t=1}^{n-p}\left(Y_t(u) - \overline{Y}(u)\right)\left(Y_{t+k}(v) - \overline{Y}(v)\right),$$

where $\overline{Y}(u)$ is the sample mean function. Also, define a non-negative operator that aggregates the dependence information across different lags

$$K(u,v) = \sum_{k=1}^{p} \int_I M_k(u,z) M_k(v,z)\, dz \tag{7}$$

and whose sample version is given by

$$\widehat{K}(u,v) = \sum_{k=1}^{p} \int_I \widehat{M}_k(u,z) \widehat{M}_k(v,z)\, dz. \tag{8}$$

If one performs an eigenanalysis of $\widehat{K}$, then the nonzero eigenvalues obtained through a bootstrap test correspond to the dynamic dimension d and the eigenfunctions associated with nonzero eigenvalues span the estimated dynamic space $\widehat{\mathcal{M}}$.

Now, we may find ourselves more comfortable on dealing with functional time series. But when it comes to probability density functions, we cannot use standard tools since the space they lie in is not a vector space. Consider the following:

Example 1. *Let $f_1(x), f_2(x)$ be two exponential probability density functions such that*

$$f_1(x) = e^{-x}, \quad f_2(x) = 2e^{-2x}, \quad x \geq 0.$$

Both f_1 and f_2 are valid PDFs, since $f_i(x) \geq 1$ and

$$\int_0^\infty f_1(x)\, dx = 1, \quad \int_0^\infty f_2(x)\, dx = 1.$$

But their sum is given by

$$f(x) = f_1(x) + f_2(x) = e^{-x} + 2e^{-2x}.$$

If we compute the integral,

$$\int_0^\infty f(x)\, dx = \int_0^\infty e^{-x}\, dx + 2\int_0^\infty e^{-2x}\, dx = 1 + 1 = 2.$$

Thus, f does not integrate to 1 and the set of PDFs is not closed under addition. Further, consider the scalar multiplication of f_1 by $\alpha = 2$. Then

$$2f_1(x) = 2e^{-x}.$$

and

$$\int_0^\infty 2f_1(x)\,dx = 2\int_0^\infty e^{-x}\,dx = 2.$$

We conclude that the set of PDFs is not closed both under addition and scalar multiplication, except for scalars equal to 1.

We can see, therefore, that the space where PDFs live is not a vector space, and we have a problem using typical tools for treating functions on Hilbert spaces. To overcome this, Hron et al. (2016) proposed a transformation into a Bayes space $\mathcal{B}^2$ of functional compositions, which is the result of a generalization of the Aitchison geometry introduced in Section 1.3, and a methodology for an adaptation of FPCA to the infinite dimensional simplex space. One of the main concerns of this research was to preserve two features of functional compositions, namely the scale invariance and the relative scale properties. The first one refers to the fact that, in Bayes spaces, two probability density functions f and g are considered equivalent if they are proportional, i.e.,

$$f = \lambda g, \quad \lambda > 0.$$

The integral constraint

$$\int_I f(x)\,dx = 1$$

selects a particular representative from the equivalence class. However, the essential information carried by the density function is not altered by scaling. In other words, multiplying a density by a positive constant does not change its relative information content. This property is known as scale invariance: only the ratios between the values of a density function matter, not their absolute scale. The latter property tells that variations in density functions must be interpreted relatively, rather than absolutely. For instance, an increase of a probability value from 0.05 to 0.1 is fundamentally different from an increase from 0.5 to 0.55, even though both changes are 0.05 in absolute terms. This implies that the analysis must be sensitive to relative changes, which motivates the use of log-ratio transformations rather than standard arithmetic differences. Thus the authors define

$$(f \oplus g)(t) = \frac{f(t)g(t)}{\int_I f(s)g(s)\,ds}, \quad (\alpha \odot f)(t) = \frac{f(t)^\alpha}{\int_I f(s)^\alpha\,ds}, \quad t \in I.$$

where $f \oplus g$ is the perturbation and $\alpha \odot f$ is the powering of two absolutely integrable density functions $f, g \in \mathcal{B}^2(I)$. These two resulting functions are probability density functions, and if we endow our space with the inner product

$$\langle f, g \rangle_{\mathcal{B}} = \frac{1}{2\eta} \int_I \int_I \ln\left(\frac{f(t)}{f(s)}\right) \ln\left(\frac{g(t)}{g(s)}\right) dt\, ds, \quad f, g \in \mathcal{B}^2(I),$$

then $\mathcal{B}^2(I)$ can be proved to be a separable Hilbert Space that is isomorphic to the Hilbert Space $L^2(I)$ through the centred log-ratio transformation given in Boogaart, Egozcue e Pawlowsky-Glahn (2014) by

$$\text{clr}(f)(t) = f_c(t) = \ln f(t) - \frac{1}{\eta} \int_I \ln f(s) ds$$

With this, the Simplicial Functional Principal Component Analysis can be performed by maximizing, over a sample $X_1, ..., X_n$,

$$\frac{1}{N} \sum_{i=1}^{N} \langle X_i, \zeta_j \rangle_{\mathcal{B}}^2 \quad \text{subject to} \quad \|\zeta_j\|_{\mathcal{B}} = 1; \quad \langle \zeta_j, \zeta_k \rangle_{\mathcal{B}} = 0, \quad k < j,$$

where $\{\zeta_j\}_{j \geq 1}, \zeta_j \in \mathcal{B}^2(I)$, are the simplicial principal components.

Another solution was given by Petersen e Müller (2016) with a mapping into a Hilbert space through a continuous and invertible map ψ that allows the implementation of standard FDA methods, with the possibility of transforming the results into the original space of densities. Two major maps are introduced: Log Quantile Density ($\psi_Q(f)$) and Log Hazard ($\psi_Q(f)$) Transformations, given by

$$\psi_Q(f)(t) = \log q(t) = -\log f(Q(t)), \quad t \in [0, 1],$$

where $q(t) = \frac{d}{dt} Q(t)$ and $Q(t)$ is the quantile function, and

$$\psi_H(f)(t) = \log\left(\frac{f(t)}{1 - F(t)}\right), \quad t \in [0, 1 - \delta],$$

where F is the cumulative distribution function. Both transformations ensure that the mapped objects lie in L^2 and both are continuous, ensuring stability of the analysis. Variations also are modeled inside the structure of density functions, avoiding artifacts caused by linear approximations. Means and variances are computed intrinsically using appropriate metrics (e.g., Wasserstein distance).

Under mild regularity assumptions, estimators of modes of variation and principal components are shown to be consistent; rates of convergence are derived both for fully observed densities and for cases where densities are estimated from data samples; optimal rates are attained when appropriate density estimators are used (e.g., modified kernel estimators).

The main results are a superior representation of variability compared to direct FPCA on densities; better interpretability of modes of variation, especially when data show horizontal variation (e.g., shifts of modes); and the fact that the methodology is applicable to regression and classification models where densities are predictors or responses. Also, a key difference about this work compared to Hron et al. (2016) is the fact that it does not rely on a specific transformation, but consider a general class of transformations independently of a metric.

5 Data analysis

6 Results

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7 Apêndice

7.1 Figuras

7.2 Tabelas