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Cramér–Karhunen–Loève representation and harmonic principal component analysis of functional time series☆

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Abstract

We develop a doubly spectral representation of a stationary functional time series, and study the properties of its empirical version. The representation decomposes the time series into an integral of uncorrelated frequency components (Cramér representation), each of which is in turn expanded in a Karhunen–Loève series. The construction is based on the spectral density operator, the functional analogue of the spectral density matrix, whose eigenvalues and eigenfunctions at different frequencies provide the building blocks of the representation. By truncating the representation at a finite level, we obtain a harmonic principal component analysis of the time series, an optimal finite dimensional reduction of the time series that captures both the temporal dynamics of the process, as well as the within-curve dynamics. Empirical versions of the decompositions are introduced, and a rigorous analysis of their large-sample behaviour is provided, that does not require any prior structural assumptions such as linearity or Gaussianity of the functional time series, but rather hinges on Brillinger-type mixing conditions involving cumulants.
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0. Introduction

Though spectral decompositions can play an important role in the statistical analysis of many classes of stochastic processes, it may not be an exaggeration to claim that in functional data

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analysis in particular, they are not simply important, but *essential*. Functional data analysis consists in drawing inferences pertaining to the law of a continuous time stochastic process $\{X(\tau); \tau \in [0, 1]\}$ with mean function and covariance operator

$$m(\tau) = \mathbb{E}[X(\tau)] \quad \text{and} \quad \mathscr{R}_0 := \mathbb{E}[(X - m) \otimes (X - m)],$$

respectively, on the basis of a collection of T (independent identically distributed) realizations of this stochastic process, $\{X_t(\tau)\}_{t=0}^{T-1}$. The process $\{X(\tau); \tau \in [0, 1]\}$ is typically modelled as a random element of a separable Hilbert space of functions, often that of square integrable complex functions defined on [0, 1], say $L^2([0, 1], \mathbb{C})$. As such, it admits a Karhunen–Loève decomposition, a spectral representation of the form

$$X(\tau) = m(\tau) + \sum_{n=1}^{\infty} \xi_n \varphi_n(\tau), \tag{1}$$

where $\{\varphi_n\}_{n=1}^{\infty}$ are the orthonormal eigenfunctions of the operator $\mathscr{R}_0$, and $\{\xi_n\}_{n=1}^{\infty}$ are the corresponding uncorrelated Fourier coefficients, $\xi_n = \int_0^1 \varphi_n(\tau)[X(\tau) - m(\tau)]d\tau$, with variance equal to the respective eigenvalue of $\mathscr{R}_0$, say λ_n. Convergence is in mean square, and can in fact be seen to be uniform over τ, provided X is continuous in mean square. The decomposition is essentially unique (assuming no multiplicities in the eigenvalues), and characterizes the law of X.

The functional principal component decomposition (1) is fundamental for a number of reasons. First and foremost, it yields a separation of variables: the stochastic part of X, represented by the countable collection $\{\xi_n\}$, is separated from the functional part, represented by the deterministic functions $\{\varphi_n\}$. Furthermore, it provides insight into the smoothness properties of the random function, which are encapsulated in the smoothness of the functions φ_n, each "relatively contributing" according to the ratio $\lambda_n / \sum_{k\geq 1} \lambda_k$. Finally, it allows for an optimal finite-dimensional approximation of the random function X, a *functional Principal Component Analysis*, in that the projection of X onto the space spanned by the first K eigenfunctions $\{\varphi_n\}_{n=1}^{K}$ provides the best K-dimensional approximation of X in mean square. As a consequence, the Karhunen–Loève representation has become both the object of and the means for much of the statistical methodology developed for functional data. It has defined what today is accepted as the canonical framework for functional data analysis and has provided a bridge allowing for a technology transfer of tools from multivariate statistics to problems of functional statistics.

As the name suggests, the Karhunen–Loève expansion can be traced back to the work of Karhunen [24] and Loève [27], the former in the context of series representations of Wiener measures and the latter in the context of linear filtering of stochastic processes. From the statistical perspective, Grenander [16] used the countable representation afforded by the expansion as a coordinate system to construct inferential procedures for random functions (perhaps marking the birth of functional data analysis; see also Grenander [17]). Large sample asymptotic properties of the empirical functional principal components, constructed on the basis of an i.i.d. sample $\{X_t(\tau); \tau \in [0, 1]\}_{t=0}^{T-1}$, were considered by Kleffe [25], who proved their consistency for the true functional principal components, and Dauxois et al. [13], who determined their asymptotic distributions. The empirical functional principal components were subsequently put to use to generalize finite-dimensional methods to the functional case, notably by Besse and Ramsay [2] and Rice and Silverman [35], leading on the one hand to a surge in methodological work on functional principal components: smooth components (e.g. Silverman [36]), higher order theory (Hall and Hosseini-Nasab [18,19]), nonparametric and conditional components (e.g. Cardot [10,11]) and components for irregularly sampled functional data (e.g. Yao et al. [38], Hall et al. [20] and

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