

Should we correct the bias in Confidence Bands for Repeated Functional Data?

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Abstract

While confidence intervals for finite quantities are well-established, constructing confidence bands for objects of infinite dimension, such as functions, poses challenges. In this paper, we explore the concept of parametric confidence bands for functional data with an orthonormal basis. Specifically, we revisit the method proposed by Sun and Loader, which yields confidence bands for the projection of the regression function in a fixed-dimensional space. This approach can introduce bias in the confidence bands when the dimension of the basis is misspecified. Leveraging this insight, we introduce a corrected, unbiased confidence band. Surprisingly, our corrected band tends to be wider than what a naive approach would suggest. To address this, we propose a model selection criterion that allows for data-driven estimation of the basis dimension. The bias is then automatically corrected after dimension selection. We illustrate these strategies using an extensive simulation study. We conclude with an application to real data.

Keywords: functional data, repeated data, confidence band, Kac-Rice formulae, bias, dimension selection

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33 **1 Introduction**

34 Functional data analysis is widely used for handling complex data with smooth shapes, finding
 35 applications in diverse fields such as neuroscience (e.g., EEG data, Zhang (2020)), psychology (e.g.,
 36 mouse-tracking data, Quinton et al. (2017)), and sensor data from daily-life activities (Jacques and
 37 Samardžić (2022)). It consists in estimating a function, which is an object of infinite dimension. It is
 38 important to accompany the function estimate with a measure of uncertainty, for example through
 39 a simultaneous confidence band. This task presents several challenges: the confidence band must
 40 control the simultaneous functional type-I error rate, as opposed to point-wise rates; it must strike
 41 a balance between being sufficiently conservative to maintain a confidence level while not being
 42 overly so as to render it meaningless; and the method used to construct this confidence band should
 43 be computationally feasible for practical application (Ramsay (2005)).

44 We consider several independent observations of the same function, i.e., noisy functional data. To
 45 analyze this noisy data, a classic approach consists in either averaging pointwise the data, applying
 46 a kernel function to smooth the noise or projecting the data onto a functional space defined by a
 47 family of functions (Kokoszka and Reimherr (2017) Chapter 3, Li, Qiu, and Xu (2022)). The pointwise
 48 empirical mean is not a function but a vector of estimated discrete points. On the other hand,
 49 with the two other approaches, the targeted function is then an approximation of the true function
 50 and obtained confidence bands are thus bands of this approximated function. In such context,
 51 several methods have been proposed to construct a confidence band that controls the simultaneous
 52 functional type-I error rate. In the case of a single individual (no repetition) but with many time
 53 points, some methods study the asymptotic distribution of the infinity norm between the targeted
 54 approximated function and its estimator, the asymptotics being in the number of time points (Hall
 55 (1991), Claeskens and Van Keilegom (2003)). These approaches only work for large datasets in
 56 time and are likely to be too conservative otherwise. For small samples, bootstrap methods have
 57 been developed to compute the confidence band (Neumann and Polzehl (1998), Claeskens and Van
 58 Keilegom (2003)), but with a high computational cost. Another approach consists in constructing
 59 confidence bands based on the volume-of-tube formula. Sun and Loader (1994) studied the tail
 60 probabilities of suprema of Gaussian random processes. This approach is based on an unbiased linear

estimator of the regression function, which corresponds to a band of the approximated targeted function. Zhou, Shen, and Wolfe (1998) used the volume-of-tube formula for estimation by regression splines. Krivobokova, Kneib, and Claeskens (2010) applied this method for the construction of confidence bands using penalized spline estimators. Bunea, Ivanescu, and Wegkamp (2011) propose a threshold-type estimator and derive error bounds and simultaneous confidence bands. In the case of several observations of the same function, Liebl and Reimherr (2023) proposed a method based on random field theory and the volume-of-tube formula, leveraging the Kac-Rice formula. Their approach introduces a quantile that varies with location, which allows to achieve their fairness property. Their confidence band uses an unbiased estimator. Unlike other methods, it does not require estimating the full covariance function of the estimator, but only its diagonal, which reduces computational time. From a practical viewpoint, Sachs, Brand, and Gabriel (2022) introduced a package to popularize simultaneous confidence bands in the context of survival analysis. Telschow and Schwartzman (2022) propose a simultaneous confidence band based on the Gaussian kinematic formula. Again, it assumes access to an asymptotically unbiased estimator of the function of interest. The coverage is thus guaranteed in the asymptotic setting after removing the bias and by targeting the approximated smoothed function. Their paper considers the non-gaussian and non-stationary cases. Wang (2022) proposed a simultaneous Kolmogorov-Smirnov confidence band by modeling the error distribution, thus avoiding the estimation of the covariance structure of the underlying stochastic process. They rely on B-splines for the estimation of the mean curve. Note that recent extensions have been proposed in Telschow et al. (2023) to construct simultaneous confidence bands, or based on conformal prediction in Diquigiovanni, Fontana, and Vantini (2022), or having a prediction goal in mind in Hernández, Cugliari, and Jacques (2024) by considering functional time series data. These different papers use approximation of the function of interest and do not deal with the non asymptotic associated bias.

We want to work in the non asymptotic setting and to propose confidence band of the original true function, not only on the approximated one (obtained by smoothing kernel or by projection). We do not work with the empirical mean estimator for two main reasons. It does not inherit functional properties, especially its regularity. Furthermore, the dimension of the empirical mean estimator is larger than the dimension of a projection or kernel estimator and this induces a larger variance and wider confidence band. Thus we focus on functional estimator.

The difference between the original function and its approximation is a functional (deterministic) bias that depends on the quality of the kernel or the projection. This bias may be neglected in the asymptotic setting where the number of observations goes to infinity, but not with finite sample sizes. It has to be taken into account in the construction of the confidence band. Both methods (kernel and projection) rely on the choice of an hyperparameter, the kernel bandwidth in the first case and the dimension of the functional projection basis in the second. The choice of this hyperparameter is crucial to control the type-I-error rate of the confidence band viewed as a band of the true function in a non-asymptotic setting. This is the question we explore in this paper.

Sun and Loader (1994) proposed a bias correction for a particular class of functions but left the smoothing parameter choice open, leading to an unusable estimator. In the nonparametric framework, the bias is approximated using the estimator of the second derivative of the underlying mean function (Xia (1998)). But in general, there is a lack of discussion on how to handle the bias of the functional estimator, even in the simple case of a functional space of finite dimension. Hard-thresholding approaches, cross-validation methods (Li, Qiu, and Xu (2022)) or model selection framework could be used to select the best dimension. However, these approaches need to be adapted to the specific case of controlling the level of a confidence band. Few references exist on this subject. For example, while the model selection paradigm has been extensively studied in the literature, in multivariate statistics or functional data analysis (e.g., Goepp, Bouaziz, and Nuel (2025), Aneiros, Novo, and Vieu

109 (2022), Basna, Nassar, and Podgórski (2022)), it has not been explored in the context of confidence
110 band construction.

111 The objective of this paper is to address the bias problem in confidence band construction for a
112 general function, in the non-asymptotic setting with respect to the number of individuals and the
113 number of time points. We adopt the point of view of projecting data onto a functional space, because
114 the functional bias is easier to study and control, than when smoothing data with a kernel. Especially,
115 when the family is an orthonormal basis, e.g., the Legendre basis (with the standard scalar product) or
116 Fourier (with another scalar product), the projection is explicit and it is possible to obtain theoretical
117 results. Moreover, the functional space offers a key advantage: it reduces the problem of inference
118 to the estimation of coefficients, for example by least squares or maximum likelihood estimation.
119 The function estimator is then simply an average after projection onto the functional base (Ramsay
120 (2005)). Our contributions are as follows:

- 121 • we disentangle the bias issue by explicitly defining the parameter of interest within the
122 approaches of Sun and Loader (1994) and Telschow et al. (2023);
- 123 • we propose a confidence band for the true function of interest, including a bias correction.
124 This provides a collection of debiased confidence bands. We also propose a criteria to select
125 the best band, by splitting the sample into two sub-samples;
- 126 • we propose a second heuristic method for selecting the dimension of the approximation space,
127 treating it as a model selection problem, with a trade-off between conservatism and confidence
128 level assurance; this approach does not correct the bias of each band of the collection but
129 selects a band with a negligible bias;
- 130 • we illustrate the proposed strategies and compare them to cross-validation or threshold ap-
131 proaches;
- 132 • we also illustrate the impact of the choice of the functional family, including non-orthonormal
133 families.

134 The paper is organized as follows: Section 2 introduces the functional regression model, the considered
135 functional family and the corresponding approximate regression models, as well as an estimator
136 defined in the finite space, along with descriptions of the error terms. In Section 3, we propose a
137 confidence band for the approximate regression function in the space of finite dimension, where the
138 dimension is fixed. Section 4 proposes a strategy to construct a confidence band for the true function.
139 This last confidence band being too conservative, Section 5 introduces a model selection criterion
140 to select the best confidence band, doing a trade-off between conservatism and confidence level
141 assurance. Section 6 illustrates the different estimating procedures of the confidence band. Section 7
142 proposes an application on real data. Section 8 ends the paper by a conclusion and discussion of
143 perspectives.

144 2 Statistical Model

145 In this paper, we consider time series as discrete measurements of functional curves. We first present
146 the general functional regression model (Section 2.1) where the regression function belongs to a
147 finite functional family of dimension L^* . In practice, this dimension L^* is unknown and we will
148 work on functional space of dimension L . The regression model on the finite family of functions is
149 presented in Section 2.2, and an estimator is proposed in Section 2.3, with a description of the error
150 terms.

151 In the rest of the paper, we consider the space $L^2([0, 1])$ with its standard scalar product $\langle f_1, f_2 \rangle =$
152 $\int_0^1 |f_1(t)f_2(t)|dt$, for $f_1, f_2 \in L^2([0, 1])$. The notation *Vect* denotes the linear span.

153 **2.1 Functional regression model**

154 Let y_{ij} be the measure at fixed time $t_j \in [a, b]$ for individual $i = 1, \dots, N$, with $j = 1, \dots, n$. The case
 155 with time observations dependent of the individuals is a natural extension of this case, but is not
 156 treated in this paper. We restrict ourselves to $[a, b] = [0, 1]$, without loss of generality. We assume
 157 these observations are discrete-time measurements of individual curves, which are independent
 158 and noisy realisations of a common function f that belongs to a functional space. Thus for each
 159 individual i , we consider the following functional regression model

$$y_{ij} = f(t_j) + \varepsilon_{ij},$$

160 where $\varepsilon_i = (\varepsilon_{i1}, \dots, \varepsilon_{in})$ is the measurement noise assuming that the ε_i are independent.

161 For each individual $i = 1, \dots, N$, we denote $y_i = (y_{i1}, \dots, y_{in})$, $t_i = (t_1, \dots, t_n)$ and $f(t_i) = (f(t_1), \dots, f(t_n))$
 162 the $n \times 1$ vectors of the observations, times and function f evaluated in t_i , respectively. We also denote
 163 $\mathbf{y} = (y_1, \dots, y_N)$ the whole matrix of observations.

164 The unknown regression function f lives in an infinite space and can not be directly estimated.
 165 First we reduce the dimension by projecting f on a function space. Let us consider L^* functions
 166 $(B_\ell^{L^*})_{1 \leq \ell \leq L^*}$ assumed to be linearly independent and the corresponding functional space $\mathcal{S}^{L^*} =$
 167 $Vect((t \mapsto B_\ell^{L^*}(t))_{1 \leq \ell \leq L^*})$. Then, for any $f \in \mathcal{S}^{L^*}$, there exists a unique vector of coefficients
 168 $(\mu_\ell^{L^*})_{1 \leq \ell \leq L^*}$ such that, for all t , $f(t) = \sum_{\ell=1}^{L^*} \mu_\ell^{L^*} B_\ell^{L^*}(t)$. The regression function f verifies the following
 169 assumption:

170 **Assumption 1.** The function f belongs to the space \mathcal{S}^{L^*} of dimension L^* . It is denoted f^{L^*} and
 171 defined as:

$$f(t) = f^{L^*}(t) = \sum_{\ell=1}^{L^*} \mu_\ell^{L^*} B_\ell^{L^*}(t).$$

172 Many functional spaces are available in the literature, as Splines, Fourier or Legendre families. We
 173 introduce the following assumption:

174 **Assumption 2.** The functional family $(t \mapsto B_\ell^{L^*}(t))_{1 \leq \ell \leq L^*}$ is orthonormal with respect to the standard
 175 scalar product $\langle \cdot, \cdot \rangle$.

176 Note that if Assumption 2 holds, one get $\mu_\ell^{L^*} = \langle f^{L^*}, B_\ell^{L^*} \rangle$ for $\ell = 1, \dots, L^*$. The Legendre family is
 177 orthonormal, the Fourier family is orthogonal for the standard scalar product (but not orthonormal),
 178 and the B-splines family is not orthogonal. We will illustrate the impact of using one family or the
 179 other in Section 6.6.

180 We also consider a functional noise through the following assumption.

181 **Assumption 3.** The sequence ε_i is functional and allows Karhunen-Loève L^2 representation: there
 182 exists a sequence of coefficients $(c_{il})_{1 \leq l}$ such that

$$\varepsilon_{ij} = \sum_{l \geq 1} c_{il} \phi_l(t_j),$$

183 where the functions $(\phi_l)_{1 \leq l}$ can be written through eigenvalues and eigenfunctions of the covariance
 184 matrix $cov(\varepsilon_{ij}, \varepsilon_{ij'})$. Practically, we assume this sum to be finite, as done for example in Chen and
 185 Song (2015): there exists L^ε such that

$$\varepsilon_{ij} = \sum_{1 \leq l \leq L^\varepsilon} c_{il} \phi_l(t_j).$$

186 We also assume that the coefficients are Gaussian: for all $i = 1, \dots, N$ and $\ell = 1, \dots, L^\varepsilon$,

$$c_{il} \sim_{iid} \mathcal{N}(0, \sigma^2).$$

187 Note that we could also work with elliptic distributions instead of the Gaussian distribution. The
188 results of the paper would be the same but require more technical details. For simplicity, we focus
189 on the Gaussian case.

190 Assumption 1 and Assumption 3 imply that each curve y_i belongs to a finite family: for $j = 1, \dots, n$,

$$y_{ij} = \sum_{\ell=1}^{L^*} \mu_\ell^{L^*} B_\ell^{L^*}(t_j) + \sum_{\ell=1}^{L^*} c_{i\ell} \phi_\ell(t_j).$$

191 As the observations are recorded at discrete time points $(t_j)_{1 \leq j \leq n}$, for $L \in \mathbb{N}$, let us denote \mathbf{B}^L the
192 matrix of $n \times L$ with coefficient in row j and column ℓ equal to $B_\ell^L(t_j)$, and the basis for the noise
193 $\Phi^{L^*} = (\phi_\ell(t_j))_{1 \leq \ell \leq L^*, 1 \leq j \leq n}$. Let us introduce $c_i = (c_{i1}, \dots, c_{iL^*})$ the $L^* \times 1$ vector. Then $\varepsilon_i = \Phi^{L^*} c_i$. The
194 vectors $y_i \in \mathbb{R}^n$ are thus independent and $y_i \sim \mathcal{N}_n(f(t_i), \sigma^2 \Sigma^{L^*})$ with $\Sigma^{L^*} = \Phi^{L^*} (\Phi^{L^*})^T$.

195 The objective of this paper is to construct a tight confidence bound for f^{L^*} using data $(y_{ij})_{ij}$. The main
196 challenge is that the true dimension L^* is unknown. In practice, we can only work with a projected
197 version on the space \mathcal{S}^L with $L \in \{L_{\min}, \dots, L_{\max}\}$. Two issues are introduced: the bias induced by
198 this projection and the choice of L . In this paper, we treat both of them in a non asymptotic setting
199 to construct confidence band with a control level.

200 In the rest of the paper, we will work with a collection of models defined by the dimension L with
201 $L \in \{L_{\min}, \dots, L_{\max}\}$, L_{\max} being chosen to be sufficiently large by the user, expecting that $L^* \leq L_{\max}$.
202 L_{\max} has to be large enough to do overfitting. We will study the functional bias and its asymptotic
203 behavior. The we will propose different strategies to choose the best dimension among the different
204 collections.

205 First, in Section 2.2 and Section 2.3, we define for a fixed L the corresponding regression model and
206 its estimator. Then Section 3, Section 4 and Section 5 will introduce the different bandwidths.

207 2.2 Approximation of the model on a finite family

208 Let $f^{L^*} \in \mathcal{S}^{L^*}$ with L^* unknown, and consider the space \mathcal{S}^L for L fixed in $\{L_{\min}, \dots, L_{\max}\}$. As \mathcal{S}^L is
209 the linear span of linearly independent functions, there is always a unique vector μ^L of coefficients
210 defining $f^L(t) = \sum_{\ell=1}^L \mu_\ell^L B_\ell^L(t) = B^L(t)\mu^L$ such that

$$f^L = \arg \min_{f \in \mathcal{S}^L} \|f^{L^*} - f\|_2^2.$$

211 If the family is orthonormal, it corresponds to the projected coefficients μ_ℓ^L :

$$\mu_\ell^L := \langle f^{L^*}, B_\ell^L \rangle.$$

212 We know that under Assumption 1, $f^{L^*,L^*} = f^{L^*}$. Moreover under Assumption 2,

$$\mu_\ell^L = \mu_\ell^{L^*} \quad \text{for } \ell = 1, \dots, \min(L, L^*).$$

213 It is interesting to note that this is not true when the basis is not orthonormal.

214 In practice, data are observed at discrete time, we consider the operator \mathbf{P}^L defined as the matrix
215 $\mathbf{P}^L = ((\mathbf{B}^L)^T \mathbf{B}^L)^{-1} (\mathbf{B}^L)^T$ of size $L \times n$. This coincides with the orthogonal projection when we deal
216 with an orthonormal basis, but this formula also holds for non orthonormal family, coming back to

217 the least square estimator on a specified family. Then we define the coefficients $\underline{\mu}^L$ which are the
 218 coefficients of μ^L approximated on the vector space, denoted \mathbf{S}^L , defined by the matrix \mathbf{B}^L .

$$\underline{\mu}^L := \mathbf{P}^L \mathbf{B}^{L*} \mu^{L*}.$$

219 Note that

- 220 • When $L \geq L^*$, when $n > L$, we have for $\ell = 1, \dots, L^*$,

$$\underline{\mu}_\ell^L = \mu_\ell^{L*}.$$

- 221 • When $L < L^*$, for $\ell = 1, \dots, L$,

$$\underline{\mu}_\ell^L \neq \mu_\ell^{L*}.$$

222 The corresponding finite approximated regression function is denoted \underline{f}^L and is defined, for all
 223 $t \in [0, 1]$, as

$$\underline{f}^L(t) = \mathbf{B}^L(t) \underline{\mu}^L.$$

224 We can observe the following, linking L, L^* and the number of timepoints n : under Assumption 1 and
 225 Assumption 2, the diagonal elements of $\mathbf{P}^L \mathbf{B}^{L*}$ are such that for $\ell = 1, \dots, \min(L, L^*)$, $[\mathbf{P}^L \mathbf{B}^{L*}]_{\ell\ell} = 1$.
 226 Moreover,

- 227 • When $n \rightarrow \infty$, for $\ell = 1, \dots, L$

$$\underline{\mu}_\ell^L \rightarrow \mu_\ell^{L*}.$$

- 228 • If $n > L^*$, then $f^{L^*} = f^{L^*, L^*} = \underline{f}^{L^*, L^*}$.

229 The last point is particularly interesting, relating n the number of timepoints to the true level L^* such
 230 that the discretized functions correspond to the true one.

231 2.3 Estimator

232 Let $L \in \{L_{\min}, \dots, L_{\max}\}$. This section presents the least square estimator of the regression function
 233 on the space of dimension L defined by the family \mathbf{B}^L and discusses its error, i.e. its bias and its
 234 behavior with respect to L and n .

235 2.3.1 Estimation of the regression function

236 When considering the estimation of the regression function f^{L^*} on the space of dimension L defined
 237 by the family \mathbf{B}^L , we do not directly estimate f^{L^*} but its projection on this finite space, which
 238 corresponds to the projected function $\underline{f}^L(t)$ and its associated coefficients $(\underline{\mu}_\ell^L)_{1 \leq \ell \leq L}$.

239 **Definition 2.1.** The vector of coefficients $(\underline{\mu}_\ell^L)_{1 \leq \ell \leq L}$ is estimated by the least square estimator $\hat{\underline{\mu}}^L$
 240 defined as:

$$\hat{\underline{\mu}}^L := \frac{1}{N} \sum_{i=1}^N \mathbf{P}^L y_i.$$

241 For a fixed $t \in [0, 1]$, the estimator of the function $\underline{f}^L(t)$ is defined by:

$$\underline{f}^L(t) = \sum_{\ell=1}^L \hat{\mu}_\ell^L B_\ell^L(t) = B^L(t) \hat{\underline{\mu}}^L. \quad (1)$$

242 Equation 1 directly implies that the estimator is thus the empirical mean of the functional approxi-
 243 mation of each individual vector of observations. Because we work with least squares estimators, we
 244 can easily study the error of estimation of $\hat{\underline{\mu}}^L$ and $\hat{\underline{f}}^L$.

245 **Proposition 2.1.** *Under Assumption 1 and Assumption 3, we have*

$$\hat{\underline{\mu}}^L \sim \mathcal{N}_L \left(\underline{\mu}^L, \frac{\sigma^2}{N} \Sigma_B^{L,L^e} \right),$$

246 where the $L \times L$ covariance matrix Σ_B^{L,L^e} is defined as $\Sigma_B^{L,L^e} := \mathbf{P}^L \Sigma^{L^e} (\mathbf{P}^L)^T$ with $\Sigma^{L^e} = \Phi^{L^e} (\Phi^{L^e})^T$.

247 Moreover, $B^L \mathbf{P}^L y_i$ is a Gaussian process with mean \underline{f}^L and covariance function $(s,t) \mapsto$
 248 $\sigma^2 B^L(s) \Sigma_B^{L,L^e} (B^L(t))^T$, and $(\hat{\underline{f}}^L - \underline{f}^L)$ is a centered Gaussian process with covariance function
 249 $C^L : (s,t) \mapsto \frac{\sigma^2}{N} B^L(s) \Sigma_B^{L,L^e} B^L(t)^T$.

250 The proof is given in Appendix.

251 Even if the estimator $\hat{\underline{f}}^L$ is defined on the functional space associated to \mathbf{S}^L , our approach consists
 252 in seeing it as an estimator of the function f^{L^*} which lies in the space \mathcal{S}^{L^*} . In that case, the error
 253 includes a functional approximation term due to the approximation of f^{L^*} on the space \mathcal{S}^L , which
 254 will be nonzero if $L \neq L^*$. It corresponds to the bias of the estimator $\hat{\underline{f}}^L$, i.e. the difference between
 255 its expectation and the true f^{L^*} . Indeed, recalling that $f^{L^*} = \underline{f}^{L^*,L^*}$, the error of estimation can be
 256 decomposed into

$$\hat{\underline{f}}^L(t) - f^{L^*}(t) = \hat{\underline{f}}^L(t) - \underline{f}^L(t) + \underline{f}^L(t) - \underline{f}^{L^*,L^*}(t) =: \text{Stat}_L(t) + \text{Bias}_L(t), \quad (2)$$

257 The first term $\text{Stat}_L(t) = \hat{\underline{f}}^L(t) - \underline{f}^L(t)$ is the (unrescaled) statistics of the model. The second term
 258 $\text{Bias}_L(t) = \mathbb{E}(\hat{\underline{f}}^L(t)) - \underline{f}^{L^*,L^*}(t)$ is the bias of the estimator $\hat{\underline{f}}^L(t)$ when estimating the true function
 259 $\underline{f}^{L^*,L^*}(t)$.

260 Let us remark that this bias is different than the bias of the estimator $\hat{\underline{f}}^L(t)$ when estimating the
 261 projected function $\hat{\underline{f}}^L = f^{L^*}$, which is 0. The two terms defined in Equation 2 are more detailed in
 262 the two next subsections.

263 2.3.2 Statistics

264 The statistics of the model, $t \mapsto \text{Stat}_L(t) = \hat{\underline{f}}^L(t) - \underline{f}^L(t)$, is a random functional quantity which
 265 depends on the estimator $\hat{\underline{f}}^L$. From Proposition 2.1, for any $t \in [0, 1]$, we define the centered and
 266 rescaled statistics $Z_L(t)$:

$$Z_L(t) := \frac{\text{Stat}_L(t)}{\sqrt{\text{Var}(\text{Stat}_L(t))}} = \frac{\hat{\underline{f}}^L(t) - \underline{f}^L(t)}{\sqrt{C^L(t,t)}} \sim \mathcal{N}(0, 1).$$

267 The covariance function can be naturally estimated using the observations y_i as

$$\hat{C}^L(s, t) = \frac{1}{N-1} \sum_{i=1}^N (B^L(s) \mathbf{P}^L y_i - \hat{\underline{f}}^L(s))(B^L(t) \mathbf{P}^L y_i - \hat{\underline{f}}^L(t)).$$

268 **2.3.3 Bias**

269 The bias is due to the fact that the estimation is potentially performed in a different (finite) space
 270 than the space where the true function \underline{f}^{*,L^*} lives. This is a functional bias, which is not random. It
 271 corresponds to the approximation of \underline{f}^{L^*} from \mathcal{S}^{L^*} to the space \mathcal{S}^L . It can be written as follows:

$$Bias_L(t) = B^L(t)\underline{\mu}_\ell^L - B^{L^*}(t)\underline{\mu}_\ell^{L^*}.$$

272 It depends on L and on the sample size through $\underline{\mu}_\ell^L$. Let us describe its behavior. When $L < L^*$ and
 273 the family is orthonormal, the approximation is the orthogonal projection and we have that

$$Bias_L(t) = \sum_{\ell=1}^L B_\ell^L(t)\underline{\mu}_\ell^L - \sum_{\ell=1}^{L^*} B_\ell^{L^*}(t)\underline{\mu}_\ell^{L^*} = \sum_{\ell=L+1}^{L^*} B_\ell^{L^*}(t)\underline{\mu}_\ell^{L^*}.$$

274 From Proposition 2.1, we can directly deduce the following proposition:

275 **Proposition 2.2.** *Under Assumption 1 and Assumption 3, the bias is, for all $t \in [0, 1]$,*

- 276 • for $L < L^*$, $Bias_L(t) \neq 0$,
 277 • for $L \geq L^*$, $Bias_L(t) = 0$.

278 Note that the bias is not 0 even when $n \rightarrow \infty$, as soon as $L < L^*$. Thus, a correct selection of the
 279 dimension L is an issue.

280 In the next section, we explain how we use this property to derive confidence bands of \underline{f}^L and f^L .

281 **3 Preliminary step: Confidence Bands of \underline{f}^L and f^L for a fixed L**

282 In this Section, we present some well known results on constructing a confidence band of \underline{f}^L and f^L .
 283 As its definition and properties are essential to construct the next steps about confidence band of
 284 f^{L^*} , we have decided to recall them in details.

285 The objective is to construct a confidence band for the two functions \underline{f}^L and f^L , based on the
 286 observations \mathbf{y} , for a given value $L \in \{L_{\min}, \dots, L_{\max}\}$. The band for \underline{f}^L enters the framework
 287 proposed by Sun and Loader (1994) which relies on an unbiased and linear estimator of the function
 288 as the estimator \underline{f}^L is an unbiased estimator of \underline{f}^L . We recall in Section 3.1 the construction of this
 289 confidence band which attains a given confidence level in a non-asymptotic setting, that is for a finite
 290 number of observations n for each individual. Then in Section 3.2, we prove that the confidence band
 291 proposed by Sun and Loader (1994) can be viewed as a confidence band for f^L with an asymptotic
 292 confidence level, the asymptotic framework being considered when $n \rightarrow \infty$.

293 **3.1 Confidence band for \underline{f}^L**

294 Consider $1 - \alpha$ a fixed confidence level. The aim is to find a function d^L such that

$$\mathbb{P}\left(\forall t \in [0, 1], \underline{f}^L(t) - d^L(t) \leq \underline{f}^L(t) \leq \underline{f}^L(t) + d^L(t)\right) = 1 - \alpha.$$

295 Consider the normalized statistics $Z_L(t)$ which is a centered and reduced Gaussian process. We want
 296 to find the quantile q^L satisfying

$$q^L = \arg \min_q \left\{ \mathbb{P} \left(\max_{t \in [0,1]} |Z_L(t)| \leq q \right) = 1 - \alpha \right\}. \quad (3)$$

Then we can take $d^L(t) = q^L \sqrt{C^L(t,t)}$. The covariance function $C^L(t,t)$ can be replaced by its estimator $\hat{C}^L(t,t)$, making the distribution a Student's distribution with $N - 1$ degrees of freedom. Thus, it only requires to be able to compute the critical value q^L .

This can be done following Sun and Loader (1994) who propose a confidence band for a centered Gaussian process. Their procedure is based on an unbiased linear estimator of the function of interest, which is the case for \underline{f}^L when we consider a band for \underline{f}^L . We recall their result in the following proposition, the computation of the value q^L is detailed thereafter. Note that the presentation of Telschow and Schwartzman (2022) is similar to the one adopted in this paper.

Theorem 3.1 (Sun and Loader (1994)). *Set Assumption 1 and Assumption 3 and a probability $\alpha \in [0, 1]$. Then, we have*

$$\mathbb{P} \left(\forall t \in [0, 1], \left| \underline{f}^L(t) - \hat{d}^L(t) \right| \leq \hat{d}^L(t) \right) = 1 - \alpha$$

with

$$\hat{d}^L(t) = \hat{q}^L \sqrt{\hat{C}^L(t,t)/N}$$

and \hat{q}^L defined as the solution of the following equation, seen as a function of q^L :

$$\alpha = \mathbb{P}(|t_{N-1}| > q^L) + \frac{\|\tau^L\|_1}{\pi} \left(1 + \frac{(q^L)^2}{N-1} \right)^{-(N-1)/2}, \quad (4)$$

with $(\tau^L)^2(t) = \partial_{12}c(t,t) = \text{Var}(Z'_L(t))$ where we denote $\partial_{12}c(t,t)$ the partial derivatives of a function $c(t,s)$ in the first and second coordinates and then evaluated at $t = s$.

We can thus deduce a confidence band of level $1 - \alpha$ for \underline{f}^L :

$$CB_1(\underline{f}^L) = \left\{ \forall t \in [0, 1], \left[\underline{f}^L(t) - \hat{d}^L(t); \underline{f}^L(t) + \hat{d}^L(t) \right] \right\}.$$

The value \hat{q}^L is defined implicitly in Equation 4 which involves the unknown and not explicit quantity $t \mapsto \tau^L(t)$. Liebl and Reimherr (2023) propose to estimate $\tau^L(t)$, for all t , by

$$\begin{aligned} \hat{\tau}^L(t) &= \left(\widehat{\text{Var}}((U^L)'_1(t), \dots, (U^L)'_N(t)) \right)^{1/2} \\ &= \left(\frac{1}{N-1} \sum_{i=1}^N \left((U^L)'_i(t) - \frac{1}{N} \sum_{j=1}^N (U^L)'_j(t) \right)^2 \right)^{1/2}, \end{aligned}$$

where $U_i^L(t) = (P^L y_i(t) - \underline{f}^L(t)) / (\hat{C}^L(t,t))^{1/2}$ and $(U^L)'_i$ is a smooth version of the differentiated function U_i^L . Then we take the L_1 -norm of $\hat{\tau}^L$.

Let us describe the behavior of \hat{d}^L :

- $\|\hat{d}^L\|_\infty$ increases with L .
- When the functions $(B_\ell^L)_{1 \leq \ell \leq L}$ form an orthonormal family, $\|\hat{d}^L\|_\infty$ increases with L until $L = L^*$ and then $\|\hat{d}^L\|_\infty$ is constant with L .

Their behavior will be illustrated with different function families in Section 6.

321 **3.2 Asymptotic confidence band for f^L**

322 Note that in the asymptotic framework $n \rightarrow \infty$, the previous definition of \hat{d}^L induces a natural
 323 asymptotic confidence band for the function f^L . Indeed, we can prove that

324 **Theorem 3.2.** Set Assumption 1 and Assumption 3 and a probability $\alpha \in [0, 1]$. Then, we have,

$$\lim_{n \rightarrow +\infty} \mathbb{P}\left(\forall t \in [0, 1], |\underline{f}^L(t) - f^L(t)| \leq \hat{d}^L(t)\right) \geq 1 - \alpha,$$

325 with $\hat{d}^L(t) = \hat{q}^L \sqrt{\hat{C}^L(t, t)/N}$ and \hat{q}^L is defined as the solution of Equation 4.

326 The proof is given in Appendix.

327 Then a confidence band for f^L at the asymptotic confidence level $1 - \alpha$ for a large number of
 328 observations n is given by

$$CB(f^L) = \left\{ \forall t \in [0, 1], \left[\underline{f}^L(t) - \hat{d}^L(t); \underline{f}^L(t) + \hat{d}^L(t) \right] \right\}.$$

329 **4 Method 1: Confidence Band of f^{L^*} by correcting the bias**

330 The function of interest is $f^{L^*} = \underline{f}^{L^*, L^*}$, rather than \underline{f}^L . Therefore, our objective is to construct a
 331 confidence band for f^{L^*} . However, an unbiased estimator of f^{L^*} is not available by definition, since
 332 the true dimension L^* is unknown. We propose instead to work with the estimator \underline{f}^L and to debias
 333 the corresponding confidence band.

334 To do this, we use the decomposition between the bias term and the statistical term, outlined in
 335 Equation 2. The idea is to bound the infinite norm of these two terms. A first strategy is to bound
 336 each term separately, then add the two bounds to construct the confidence band. However, this
 337 approach tends to produce a band that is too large and too conservative. This is because applying the
 338 infinite norm to each term before bounding them does not take into account the functional nature of
 339 the two terms.

340 A second strategy is to retain the functional aspect by bounding the infinity norm of the sum of the
 341 two functional terms. This approach is detailed in this section.

342 In Section 4.1, we first rewrite the band as a band around $\underline{f}^L(t)$. We need to estimate the band bound
 343 and the bias. To do this, we divide the sample into two sub-samples. This choice is not ideal because
 344 it increases the variability of the estimators. But at least, it provides independence between the
 345 estimators of the two quantities, which makes it possible to establish the theoretical coverage of the
 346 final band. More precisely, we use a first subsample y^1 to estimate the bound defined in Section 3. A
 347 second subsample y^2 is used to estimate the bias term (without the infinite norm). This results in a
 348 pointwise correction of the bias, and the final confidence band is centered around $\underline{f}^{L_{\max}, L^*}$.

349 This procedure provides a collection of confidence bands, for $L \in \{L_{\min}, \dots, L_{\max}\}$ with variable width.
 350 Then, in Section 4.2, we propose a criterion to select the “best” band by minimizing its width. We
 351 discuss the band thus obtained at the end of the section and its limits.

352 **4.1 Construction of the band of f^{L^*} for a given L**

353 We introduce two independent sub-samples y^1 and y^2 of y of length N_1 and N_2 such that $N_1 + N_2 = N$.

354 We use the first sub-sample \mathbf{y}^1 to calculate $\hat{\underline{f}}_1^L(t)$, an estimator of $\underline{f}^L(t)$ and a functional bound
 355 denoted \hat{d}_1^L that controls the bias term $\underline{f}^L(t) - \hat{\underline{f}}_1^L(t)$. This bound is defined in Section 3 applied on
 356 \mathbf{y}^1 , for a given level α , such that:

$$\mathbb{P}\left(\forall t \in [0, 1], -\hat{d}_1^L(t) \leq \underline{f}^L(t) - \hat{\underline{f}}_1^L(t) \leq \hat{d}_1^L(t)\right) = 1 - \alpha. \quad (5)$$

357 Next, we need to control the bias $Bias_L(t) = \underline{f}^L(t) - f^{L^*}(t)$. Recall that when L_{\max} is sufficiently large
 358 and $n > L_{\max}$, we have $f^{L^*} = \underline{f}_{\max}^{L^*}$. We therefore need to control the $Bias_L(t) = \underline{f}^L(t) - \underline{f}_{\max}^{L^*}(t)$.
 359 It would be tempting to replace $Bias_L(t)$ by its estimation based on the second sample \mathbf{y}^2 , but this
 360 would introduce an estimation error that we also need to control, in the same spirit as what is
 361 done in Lacour, Massart, and Rivoirard (2017). We can again use Section 3 to compute the function
 362 $\hat{d}_2^{L_{\max}}(t)$ on the sample \mathbf{y}^2 , and the functional estimators $\hat{\underline{f}}_2^L(t)$ and $\hat{\underline{f}}_2^{L_{\max},L^*}(t)$ of $\underline{f}^L(t)$ and $\underline{f}_{\max}^{L^*}(t)$,
 363 respectively. This allows us to construct the following band for $\underline{f}^L(t) - \underline{f}_{\max}^{L^*}$ for a confidence level
 364 $1 - \beta$,

$$\mathbb{P}\left(\forall t \in [0, 1], -\hat{d}_2^{L_{\max}}(t) \leq \underline{f}_{\max}^{L^*}(t) - \underline{f}^L(t) - (\hat{\underline{f}}_2^{L_{\max},L^*}(t) - \hat{\underline{f}}_2^L(t)) \leq \hat{d}_2^{L_{\max}}(t)\right) = 1 - \beta. \quad (6)$$

365 Combining Equation 5 and Equation 6, we can provide a debiased confidence band of $f^{L^*}(t)$.

366 **Proposition 4.1.** *Let us define*

$$\begin{aligned} \hat{\theta}_1^L(t) &:= -\hat{d}_1^L(t) - \hat{d}_2^{L_{\max}}(t) + \hat{\underline{f}}_2^{L_{\max},L^*}(t) - \hat{\underline{f}}_2^L(t) \\ \hat{\theta}_2^L(t) &:= \hat{d}_1^L(t) + \hat{d}_2^{L_{\max}}(t) + \hat{\underline{f}}_2^{L_{\max},L^*}(t) - \hat{\underline{f}}_2^L(t), \end{aligned}$$

367 where $\hat{d}_1^L(t)$ is defined on sample \mathbf{y}^1 by Equation 5 for a level α and $\hat{d}_2^{L_{\max}}(t)$ is defined on sample \mathbf{y}^2 by
 368 Equation 6 for a level β . Then we have

$$\mathbb{P}\left(\forall t \in [0, 1], \hat{\theta}_1^L(t) \leq f^{L^*}(t) - \hat{\underline{f}}_1^L(t) \leq \hat{\theta}_2^L(t)\right) \geq 1 - \alpha\beta.$$

369 The proof is given in Appendix.

370 This defines a confidence band which can be defined either around $\hat{\underline{f}}_1^L$:

$$CB_2(\underline{f}^{L^*}) = \left\{ \forall t \in [0, 1], \left[\hat{\underline{f}}_1^{L,L^*}(t) + \hat{\theta}_1^L(t); \hat{\underline{f}}_1^{L,L^*}(t) + \hat{\theta}_2^L(t) \right] \right\}$$

371 or around $\hat{\underline{f}}_2^{L_{\max},L^*}$:

$$CB_2(\underline{f}^{L^*}) = \left\{ \forall t \in [0, 1], \left[\hat{\underline{f}}_2^{L_{\max},L^*}(t) + \bar{\theta}_1^L(t); \hat{\underline{f}}_2^{L_{\max},L^*}(t) + \bar{\theta}_2^L(t) \right] \right\}.$$

372 with $\bar{\theta}_1^L(t) = \hat{\underline{f}}_1^L(t) - \hat{\underline{f}}_2^{L,L^*}(t) - \hat{d}_1^L(t) - \hat{d}_2^{L_{\max}}(t)$ and $\bar{\theta}_2^L(t) = \hat{\underline{f}}_1^L(t) - \hat{\underline{f}}_2^{L,L^*}(t) + \hat{d}_1^L(t) + \hat{d}_2^{L_{\max}}(t)$.

373 *Remark 4.1.* The two functions $\hat{d}_1^L(t)$ and $\hat{d}_2^{L_{\max}}(t)$ are of the same order because they are constructed
 374 using the same approach. They depend on the length of the samples. To obtain the thinnest band,
 375 the best strategy is to divide the sample in two sub-samples of equal length $N_1 = N_2 = N/2$.

376 The behavior of \hat{d}_1^L was described in Section 3. Let us describe the behavior of $\hat{d}_2^{L,L_{\max}}$:

- 377 • $\|\hat{d}_2^{L,L_{\max}}\|_\infty$ decreases with L .
- 378 • When $L > L^\varepsilon$, $\|\hat{d}_2^{L,L_{\max}}\|_\infty$ is constant with L and the probability in Equation 6 is equal to 1.
- 379 • When $L^* < L < L^\varepsilon$, $\|\hat{d}_2^{L,L_{\max}}\|_\infty$ is constant with L when the functions B_t^L form an orthonormal family. Otherwise, the behavior is erratic.

381 This means that when the band defined in Proposition 4.1 is calculated for $L > L^\varepsilon$, the confidence
382 level is $1 - \alpha$ instead of $1 - \alpha\beta$.

383 The advantage of this approach is that the band bias is corrected and the level for the true function f^{L^*}
384 is guaranteed when L^ε is large. This was the main aim of the paper. The main limit of this approach
385 is that the band is constructed with samples with half sizes, leading to less precision. This will be
386 illustrated in Section 6. Nevertheless, this method gives finer confidence bands than cross-validation,
387 and with the right level of confidence.

388 A natural question is then the choice of the dimension L . This is the purpose of the next section.

389 4.2 Influence of L

390 This approach produces a collection of debiased confidence bands for different values of L . The
391 confidence bands have different widths but the same confidence level $1 - \alpha\beta$. It is therefore natural to
392 want to select one of them. This means we want to select the best dimension L among the collection
393 $\{L_{\min}, \dots, L_{\max}\}$. We need to define what “best” means. It is quite intuitive to want to focus on the
394 finest band, fine in the sense of a certain norm. Here we consider the infinite norm of the width
395 of the confidence band. This gives preference to smooth bands. We therefore define the following
396 criteria for selecting L .

$$\hat{L} = \arg \min_L \left\{ \sup_t |\hat{\theta}_2^L(t) - \hat{\theta}_1^L(t)| \right\} = \arg \min_L \left\{ \sup_t |\hat{d}^L(t) + \hat{d}^{L,L_{\max}}(t)| \right\}. \quad (7)$$

397 This global approach guarantees that each band of the collection is debiased and then the dimension
398 is selected. It will be illustrated in Section 6.

399 In the next section, instead of debiasing each band, we employ another strategy focusing on the
400 construction of a selection criteria that will guarantee that the bias is negligible.

401 5 Method 2: Selection of the best confidence band with a criteria 402 taking into account the bias

403 In this section, we propose a new method in the non asymptotic setting to provide a confidence band
404 of f^{L^*} without correction the bias but taking it into account in the selection procedure.

405 Our method uses the collection of confidence bands defined in Section 3. Instead of correcting their
406 bias, the strategy is to propose a selection criterion that is a trade-off between this bias and the
407 dimension of the basis. To do this, we propose a new heuristic criterion linked to the definition of
408 the band itself, considering the estimation of the band as the estimation of a quantile of a certain
409 empirical process. The criterion is inspired by model selection tools for choosing the best dimension
410 L . In the following, we assume that L_{\max} is large enough such that $\underline{f}^{L_{\max}, L^*} = f^{L^*}$.

411 We work on the quantile q^L introduced in Equation 3, its oracle version q^{L^*} for level L^* and its
412 estimate \hat{q}^L . All are scalars, belonging to a collection indexed by $L \in \{L_{\min}, \dots, L_{\max}\}$. A natural

413 criterion for choosing the best L is that the estimator \hat{q}^L minimizes the quadratic error $\mathbb{E}(\|q^{L^*} - \hat{q}^L\|^2)$.
 414 However, this quadratic error is unknown as q^{L^*} is unknown. We cannot use it directly.

415 Instead, we study $\|\hat{q}^{L_{\max}} - \hat{q}^L\|^2$. While the theoretical quadratic error $\mathbb{E}(\|q^{L^*} - \hat{q}^L\|^2)$ decreases when
 416 $L < L^*$ and increases when $L > L^*$, the $\|\hat{q}^{L_{\max}} - \hat{q}^L\|^2$ approximation to this error always decreases
 417 when $L > L^*$, as illustrated in Section 6.

418 We see a behavior similar to a bias, high when the dimension is small, and small when the dimension
 419 is large. Selecting a dimension using this criterion will always overfit the data. We therefore propose
 420 to penalize this quantity by the dimension L divided by the sample size N , as usual in model selection
 421 criteria. To do this, we introduce a regularisation parameter $\lambda > 0$ which balances the two terms. A
 422 natural criterion to select the best L is then

$$\widetilde{\text{crit}}(L) = \|\hat{q}^{L_{\max}} - \hat{q}^L\|^2 + \lambda \frac{L}{N}.$$

423 Then we define

$$\tilde{L} = \arg \min_L \widetilde{\text{crit}}(L),$$

424 and take the band centered around $\underline{f}^{\tilde{L}, L^*}$:

$$CB_3(\underline{f}^{L^*}) = CB_1(\underline{f}^{\tilde{L}, L^*})$$

425 This criterion is illustrated in Section 6.5. We also compare with two other standard approaches,
 426 heuristic as well, namely the cross-validation approach used to select the dimension L which mini-
 427 mizes the reconstruction error, and a thresholding method which keeps the higher dimension L with
 428 large enough coefficients. These two methods are less oriented to the objective of controlling the
 429 level of the selected confidence band.

430 6 Simulation study

431 In this section, we illustrate the different statements provided along the paper on generated data. First,
 432 in Section 6.1, we describe the generating data process and illustrate the linear estimator considered
 433 in this paper. In Section 6.2, we illustrate the first confidence band, for a fixed level, as introduced in
 434 Section 3. Then, we illustrate the debiased confidence band in Section 6.3, and discuss the model
 435 selection criterion in Section 6.4, comparing both of them with state-of-the-art methods in Section 6.5.
 436 We finally study the generalization of the method out of the class of models in Section 6.6.

437 6.1 Generating data process

438 To illustrate the model, we simulate a regression functional model with $n = 40$ regular timepoints per
 439 individual and $N = 25$ individuals. In Figure 1, the function f (black curve) belongs to the Fourier
 440 (resp. Legendre and Spline) family with $L^* = 7$ and the noisy individual observations $(y_{ij})_{1 \leq i \leq N, 1 \leq j \leq n}$
 441 (grey curves) have a functional noise in dimension $L^\varepsilon = 15$, also in the Fourier (resp. Legendre and
 442 Spline) family on the left plot (resp. middle and right).

443 6.2 Confidence band for a fixed level

444 The general band for f^L derived in Theorem 3.1 is illustrated on Figure 2. It displays on the top row
 445 several functional data generated under either the Fourier family (left), Legendre (middle) or Spline
 446 (right), on the middle row the confidence bands of \underline{f}^L for different values of $L \in \{3, 5, 7, 11\}$ and 15,

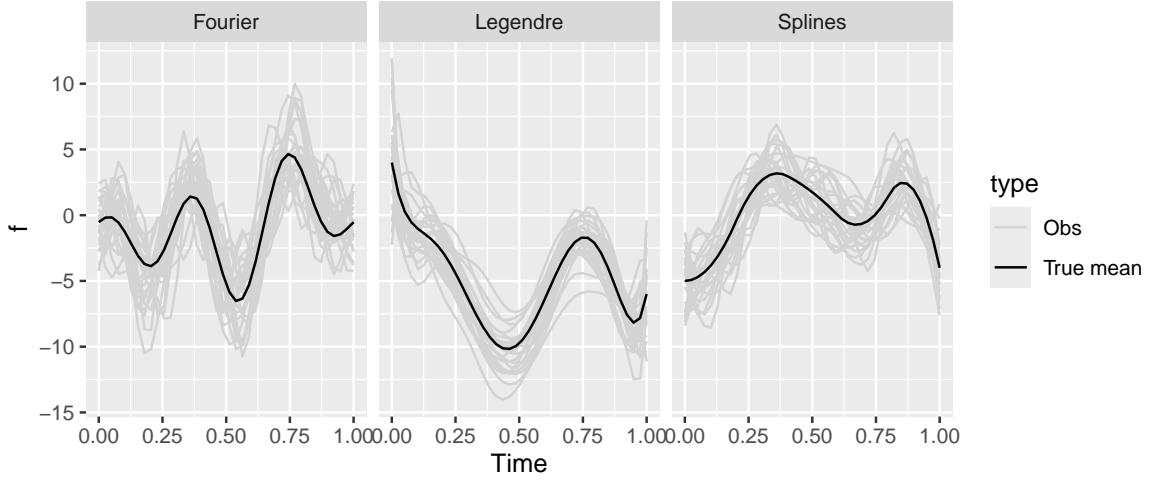


Figure 1: Functional regression with different bases. We generate a regression functional model using three different basis families: Fourier (left), Legendre (middle), and Splines (right). The black curve represents the true mean function, while the gray curves show individual noisy observations.

and on the bottom row the bound \hat{d}^L . On the middle row, the true functions f^L are displayed in black and the confidence bands in color. The bands are very precise for each L . The behavior of \hat{d}^L increases with L . As d^L can be seen as a variance, $\hat{d}^L(t)$ is larger on the boundary of the time domain, as there are less observations near 0 and 1.

We also evaluate numerically the levels of the obtained confidence bands. For this, 1000 datasets are simulated, the confidence band is estimated for each of them. The empirical confidence level is then evaluated as the proportion of confidence bands that contain the true function over 5000 test timepoints. Table 1 presents the empirical confidence levels for different values of L and several sample sizes $n \in \{40, 150\}$, and $N \in \{10, 25, 60\}$, and for the 3 basis. When $N = 25$ and $N = 60$, the level is the expected one whatever the value of L . We will see in the next sections that this will not be the case for the debiased confidence band. When $N = 10$, the level is too small, especially when L is large. This might be due to the the large number of parameters to be estimated in the covariance matrix, with a small number of observations N .

6.3 Method 1: confidence bands by correcting the bias

We illustrate the confidence band of f^{L^*} given in Proposition 4.1. In Figure 3, top row, we plot the confidence bands obtained for different dimensions $L \in \{3, 5, 7, 11, 15\}$ with Fourier, Legendre and Splines families and $\alpha = \beta = \sqrt{0.05} \approx 0.22$. We can see that all the confidence bands are alike. Especially, they are unbiased, even for $L = 3$. A larger dimension L provides a smoother band. On the middle and bottom rows of Figure 3, we illustrate the two terms that enter the confidence band, $t \mapsto \hat{d}_1^L(t)$ and $t \mapsto \hat{d}_2^{L,L_{\max}}(t)$. Their behavior is the same along time. The function $\hat{d}_1^L(t)$ can be seen as a variance, this is why it is larger near 0 and 1 where there are less observations. The function $\hat{d}_2^{L,L_{\max}}(t)$ is smaller than $\hat{d}_1^L(t)$ because it controls the remaining rest after the projection. Note that as expected when $L > L^\varepsilon$, $\hat{d}_2^{L,L_{\max}}(t)$ is close to 0. As explained before, the influence of L is not the same for the two functions. When L increases, $\hat{d}_1^L(t)$ increases while $\hat{d}_2^{L,L_{\max}}(t)$ decreases.

In Table 2, we simulate 1000 repeated datasets with the Legendre family and with two sample sizes $n = 40$ and $n = 150$ and $N = 25$. For each dataset, we compute the confidence band defined in Proposition 4.1 with a theoretical confidence level of $1 - \alpha\beta = 0.95$ and for different values of L .

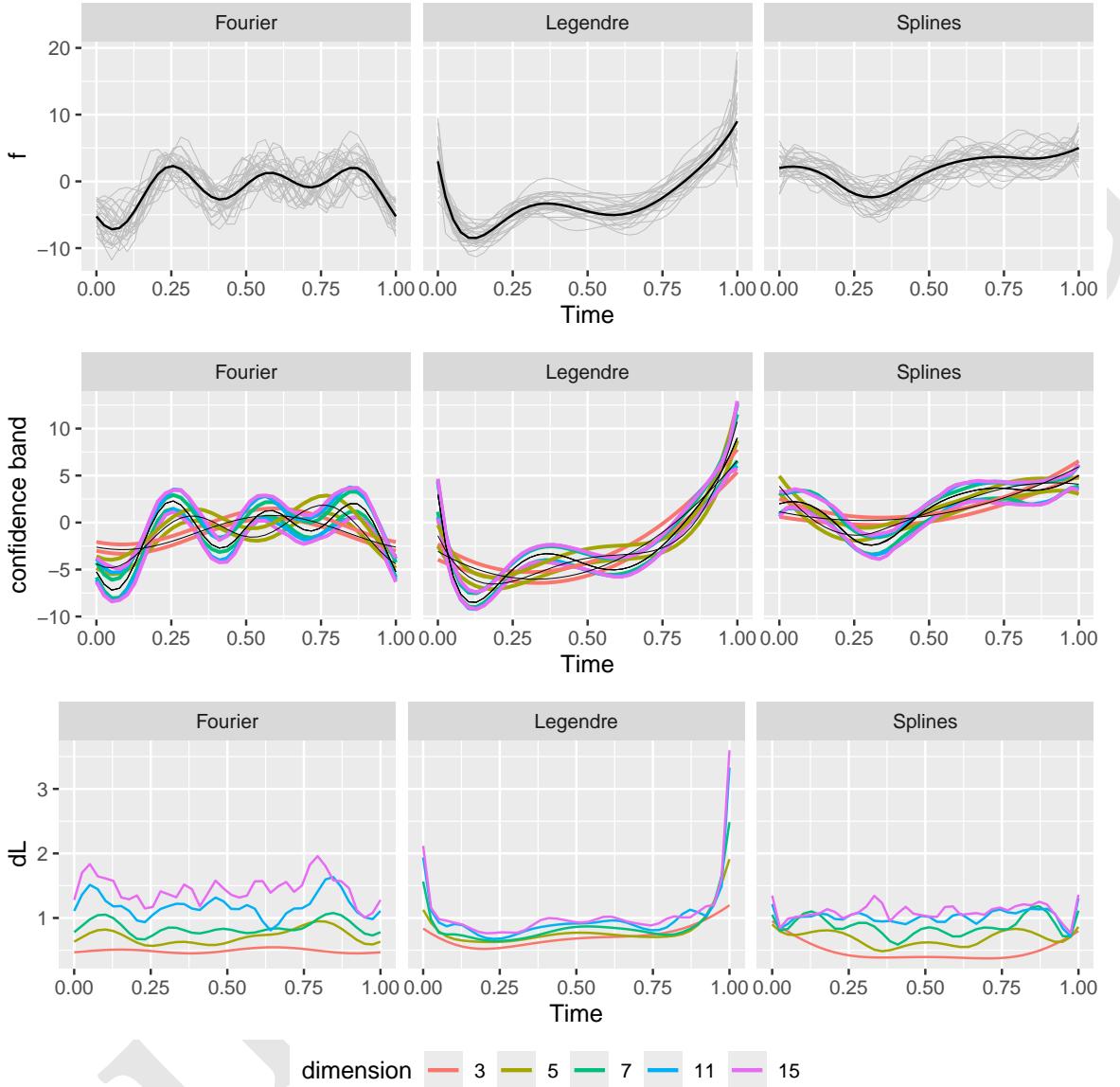


Figure 2: Confidence bands for f^L . For the three basis families (Fourier, on the left, Legendre, on the middle, and Splines on the right) we display: (top row) the observed functional data; (middle row) the estimated confidence bands for increasing values of L (3, 5, 7, 11 and 15); and (bottom row) the associated bound dL .

Table 1: Empirical coverage of CB for different basis families. The empirical confidence level of the confidence band CB is estimated over 1000 repetitions, for alpha = 0.05. Confidence bands are calculated with the Fourier (top), Legendre (middle) and Splines (bottom) basis families. Each row corresponds to a different number of basis functions L, and each column to a different pair of sample sizes (n,N).

L	n/N					
	40/10	150/10	40/25	150/25	40/60	150/60
3	0.930	0.933	0.939	0.942	0.952	0.951
5	0.921	0.913	0.927	0.927	0.950	0.951
7	0.926	0.926	0.931	0.930	0.948	0.950
11	0.921	0.911	0.933	0.933	0.951	0.951
15	0.915	0.901	0.926	0.927	0.943	0.943
L	n/N					
	40/10	150/10	40/25	150/25	40/60	150/60
3	0.926	0.928	0.935	0.937	0.947	0.945
5	0.925	0.926	0.928	0.937	0.946	0.943
7	0.924	0.929	0.927	0.937	0.923	0.939
11	0.927	0.924	0.923	0.931	0.936	0.942
15	0.929	0.929	0.931	0.935	0.942	0.944
L	n/N					
	40/10	150/10	40/25	150/25	40/60	150/60
3	0.929	0.930	0.927	0.931	0.936	0.939
5	0.921	0.917	0.943	0.944	0.941	0.946
7	0.911	0.915	0.939	0.942	0.952	0.950
11	0.913	0.911	0.948	0.951	0.952	0.949
15	0.903	0.900	0.950	0.946	0.952	0.955

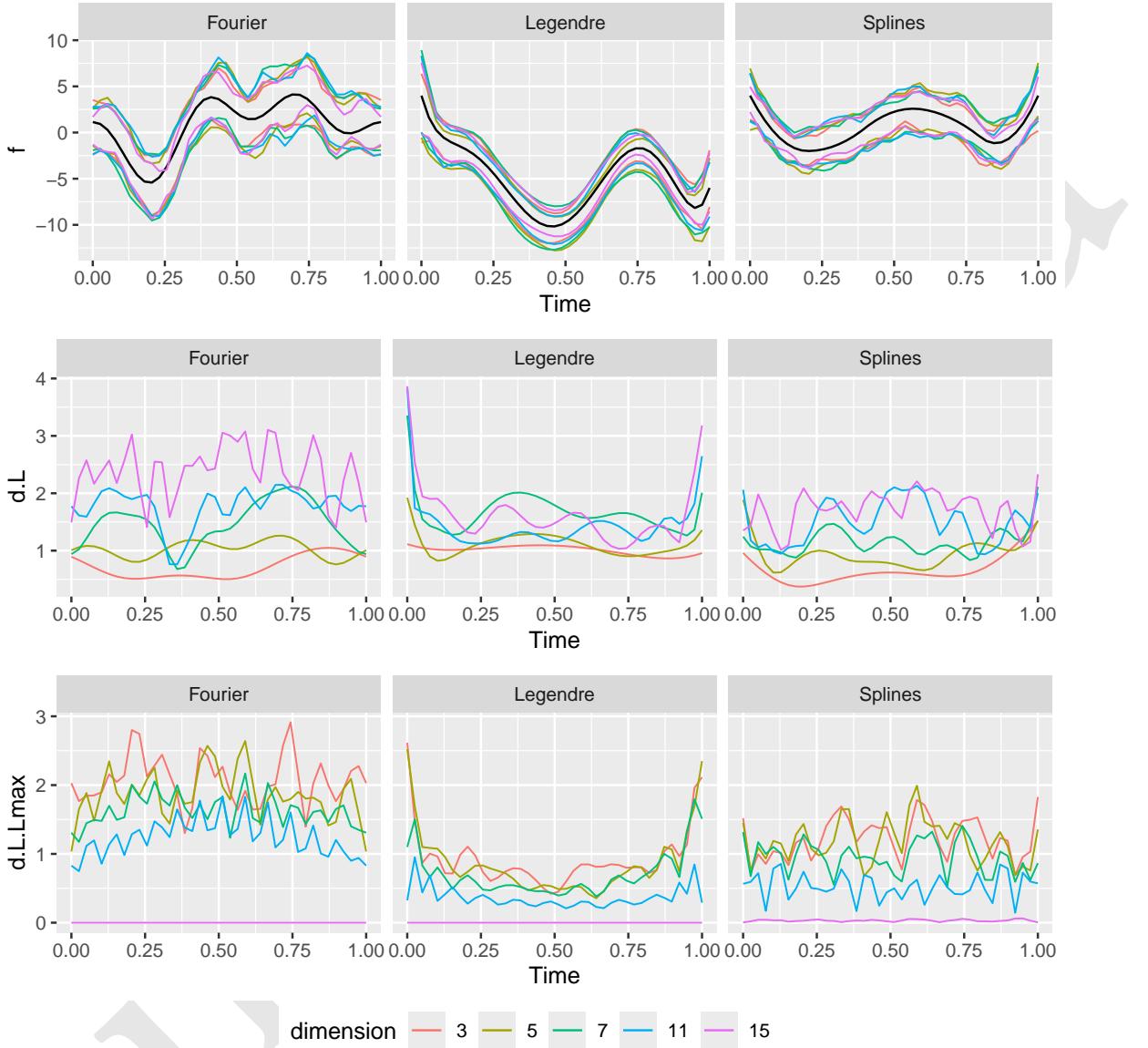


Figure 3: Visualization of confidence bands by correcting the bias. For a given dataset, we plot several confidence bands (top row), functions dL (middle row) and dLL_{\max} (bottom row). Bands and functions are estimated with Fourier (left column), Legendre (middle column) and Spline (right column) basis and several dimensions L (3, 5, 7, 11, 15), and $L_{\max} = 25$.

Table 2: Empirical coverage of CB2. The table reports the empirical level of confidence of the proposed confidence band CB2, computed for various values of L (rows) and n (columns), with fixed N=25, and various basis (top: Fourier, middle: Legendre, bottom: Splines). The nominal confidence level is set to 0.05, using parameters alpha=beta=0.2, such that the combined coverage is 1-0.95.

L	n	
	40	150
3	0.958	0.958
5	0.966	0.966
7	0.980	0.980
11	0.983	0.983
15	0.723	0.723

L	n	
	40	150
3	0.925	0.925
5	0.948	0.948
7	0.951	0.951
11	0.923	0.923
15	0.747	0.747

L	n	
	40	150
3	0.953	0.953
5	0.973	0.973
7	0.963	0.963
11	0.910	0.910
15	0.728	0.728

474 Then the confidence level is approximated as the proportion of confidence bands containing the true
 475 function f over 5000 test timepoints. Remark that when $L < L^\varepsilon$, the level is the expected one, that
 476 is 0.95. When $L > L^\varepsilon$, the level is no more ensured, as explained before. Indeed the term $d^{L,L^{\max}}$ is
 477 mainly equal to 0 when L^{\max} is large enough, and the level is close to $1 - \alpha$ instead of $1 - \alpha\beta$. This is
 478 not the case for the band in Section 3, as this is due to the correction of the bias.

479 We illustrate the different terms involved in Equation 7 in Figure 4: we plot for a given dataset,
 480 the infinity norm of the width of the band $\hat{d}^L(t) + \hat{d}^{L,L^{\max}}(t)$ (top), of $\hat{d}^L(t)$ (middle) and $\hat{d}^{L,L^{\max}}(t)$
 481 (bottom) functions obtained with the Fourier (left column), Legendre (middle column) and Spline
 482 (right column) basis. As already said, $\|\hat{d}^L\|_\infty$ increases with L while $\|\hat{d}^{L,L^{\max}}\|_\infty$ decreases (and is zero
 483 when $L > L^\varepsilon$). The width of the band wrt L does not have a U-shape, as expected. It is thus difficult
 484 to minimize this criterion and the selection of \hat{L} is thus not stable. But again, whatever the value
 485 of \hat{L} , the corresponding band is debiased in the collection. We will see in the next sections that its
 486 width is smaller than standard approaches. The performance of the selection is also illustrated in the
 487 next section.

488 6.4 Method 2: a model selection criterion to take into account the bias

489 In Figure 5, we illustrate the behavior of the selection criterion introduced in Section 5 on simulated
 490 data, with $\lambda \in \{0, 0.5, 1, 2\}$ for the three basis. We can see that \tilde{L} is overestimated. When considering

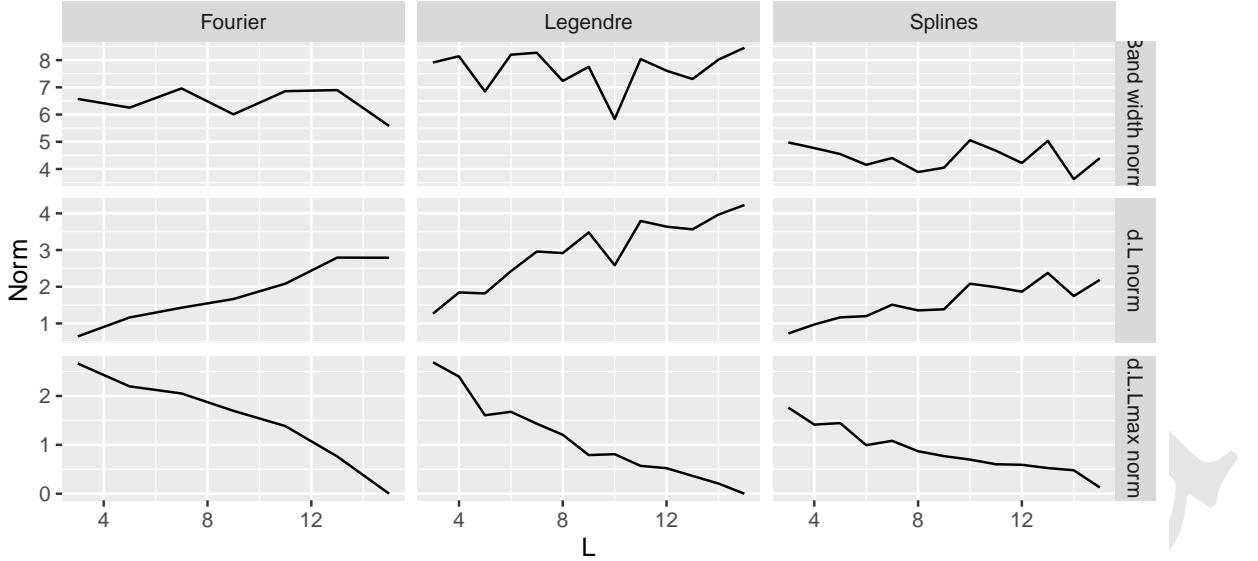


Figure 4: Norm of the confidence band width and associated bounds. For a given dataset, we compute: (top row) the norm of the width of the confidence band; (middle row) the norm of the function dL ; and (bottom row) the norm of the function $dLLmax$, for various dimensions L . Results are shown for the Fourier (left column), Legendre (middle column), and Splines (right column) basis families.

491 nested spaces, it ensures that \tilde{L} tends to be larger than L^* and thus the confidence band is automatically
 492 unbiased.

493 6.5 Comparison of the methods with the state-of-the-art

494 We evaluate the performance of the two selection criteria introduced in this paper, and compare
 495 the two strategies CB_2 and CB_3 with some standard approaches. More precisely, we simulate 1000
 496 repeated datasets. The different confidence bands and the norm of their widths are computed for
 497 several L . We apply the selection criteria and plot the distribution of the estimated dimension in
 498 Figure 6, for the three basis families, for several model selection criteria: \hat{L} , \tilde{L} , cross validation and
 499 hard thresholding. The dimension \hat{L} is almost always larger than the true $L^* = 7$. The fact that it is
 500 larger is not a problem because the selected band is unbiased and has the correct level as soon as
 501 L^* is large. However, the criterion tends to select a band that is (too) smooth. We can see that the
 502 selected dimension \tilde{L} is smaller in distribution, and closer to the true value than \hat{L} . In addition, as we
 503 then use the confidence band of Section 3, the confidence level is guaranteed to be as expected. The
 504 model selected by cross validation is rather good, for all the basis considered. On the other hand, the
 505 model selected by hard thresholding is not good, particularly for a non orthonormal basis.

506 The reformulation of the band around $\underline{f}_2^{L_{\max}, L^*}$ is close to the band presented in Section 3 for
 507 $L = L_{\max}$, that is a band centered around $\underline{f}^{L_{\max}, L^*}$. A natural question is to understand what is
 508 the gain by doing so instead of using the band from Section 3 with $L = L_{\max}$, namely the band
 509 $\left[\underline{f}^{L_{\max}, L^*}(t) - \hat{d}^{L_{\max}}(t); \underline{f}^{L_{\max}, L^*}(t) + \hat{d}^{L_{\max}}(t) \right]$. To do that, we have to understand the behavior of the
 510 different terms. As it is difficult to compare theoretically the width of the two bands, we compare
 511 them using simulations. For 1000 repeated datasets, we compute several confidence bands: the CB_1
 512 band constructed in Section 3 with L_{\max} , the CB_2 band defined in Proposition 4.1 with \hat{L} , the CB_3
 513 band defined in Section 5 with \tilde{L} and the ideal (and not accessible) band constructed in Section 3 with
 514 the true L^* . In Figure 7, we present boxplots of the norms of the band width with \hat{L} , L_{\max} , L^* and

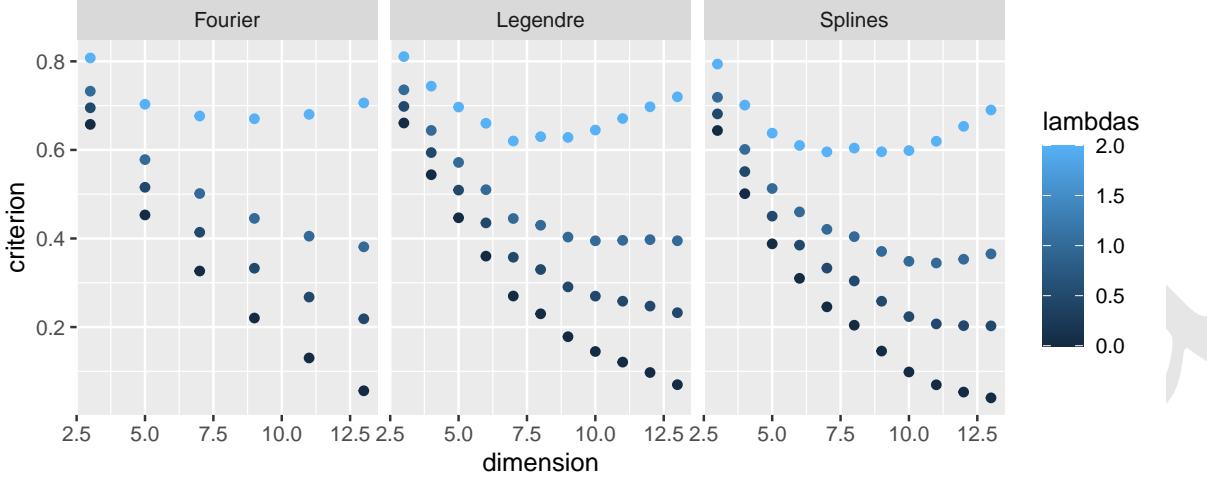


Figure 5: Behavior of selection criteria as a function of model dimension. For a given simulated dataset, we display the evolution of the selection criteria with respect to the dimension L , for several values of the regularization parameter λ . Results are shown for the Fourier (left), Legendre (middle), and Splines (right) basis families.

Table 3: Comparison with the state-of-the-art for the empirical confidence level. The table reports the performance of the proposed confidence band CB3, estimated over 1000 repetitions, for various model selection criteria and competitive methods (rows) and for various basis families (columns). Results are shown for $\alpha=0.05$, with $n=40$ and $N=25$.

model	Fourier	Legendre	Splines
Lstar	0.931	0.932	0.940
Lmax	0.926	0.932	0.949
Lhat	0.972	0.924	0.904
Ltilde	0.933	0.926	0.926
LL0	0.895	0.922	0.901
LCV	0.913	0.918	0.831
Mean	0.926	0.932	0.950
FFSCB	0.922	0.941	0.950

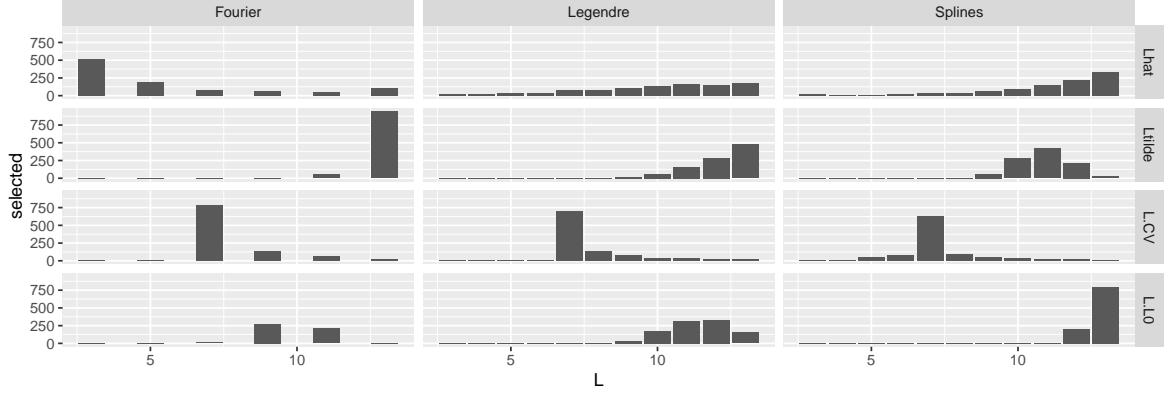


Figure 6: Distribution of the selected model dimension across selection methods. Based on 1000 simulated datasets, we report the distribution of the estimated dimension L for four model selection methods: from top to bottom — the debiased confidence band CB2 with \hat{L} , the band CB3 with \tilde{L} , cross-validation, and hard-thresholding. The true model dimension is $L_{\text{star}} = 7$.

515 \tilde{L} . We also use the empirical mean and the method FFSCB Liebl and Reimherr (2023). The width of
 516 the confidence band with the true L^* is smaller, which is expected but unfortunately not achievable.
 517 The width of the confidence band CB_1 is smaller than that of the band CB_2 . This can be explained by
 518 the fact that we estimate two different quantities, on smaller datasets, for more conservative levels
 519 ($1 - \alpha$ and $1 - \beta$ respectively) in order to finally achieve the confidence level of $1 - \alpha\beta$. This also
 520 explains why the cross validation and hard-thresholding methods, which also divide the sample into
 521 two parts, do not give good results either. The model given by the heuristic model selection criterion
 522 $\widetilde{\text{crit}}$ achieves good performance. Note that the width of the selected model \tilde{L} is better than the width
 523 of the confidence band with a large level L_{\max} , which one should have used to avoid model selection.
 524 The empirical mean and the band given by FFSCB are a bit larger.

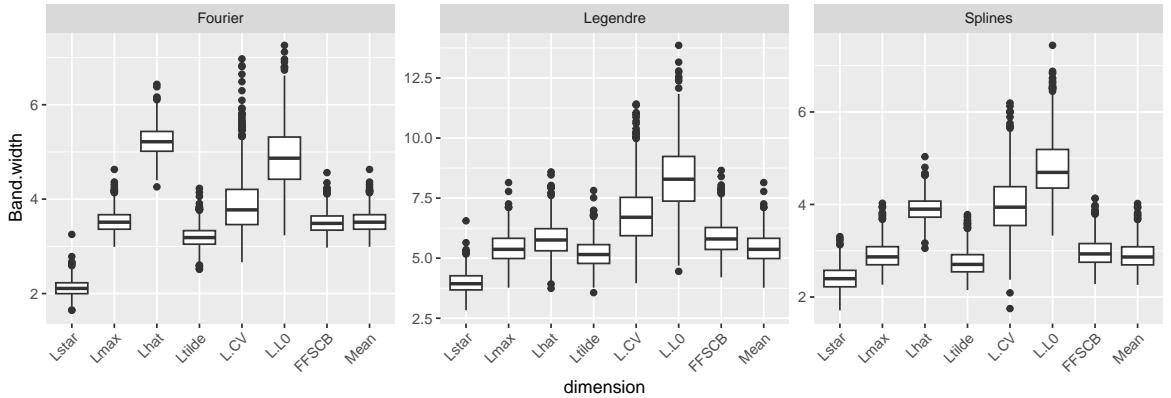


Figure 7: Width of the confidence bands accross selection methods. Boxplots show the distribution of the confidence band width over 1000 repetitions, for the dimension selected by the various criteria introduced in this paper (as well as standard baselines). Results are shown for the Fourier (left), Legendre (middle), and Splines (right) basis families.

525 6.6 Generalization out of the model

526 We now illustrate the behaviour of the bands when the basis used for estimation is poorly specified.
 527 We simulate 1000 data sets with a spline basis and estimate the confidence bands with the Fourier
 528 and Legendre basis, for different values of n and N . The coverage rates are presented in Table 4.

Table 4: Empirical coverage of confidence bands under model misspecification. The empirical confidence level is estimated over 1000 repetitions. Data are generated using a Splines basis, while confidence bands are computed using the Fourier (top) and Legendre (bottom) basis families. Each row corresponds to a different value of L, and each column to a different pair of sample sizes (n,N).

L	n/N			
	50/10	150/10	50/40	150/40
5	0.057	0.057	0.016	0.017
7	0.113	0.107	0.042	0.039
11	0.232	0.205	0.096	0.077
15	0.298	0.254	0.153	0.118

L	n/N			
	50/10	150/10	50/40	150/40
5	0.133	0.142	0.031	0.035
7	0.684	0.679	0.415	0.429
11	0.914	0.910	0.939	0.940
15	0.916	0.912	0.951	0.951

Table 5: Empirical coverage of confidence bands across selection methods under model misspecification. The empirical confidence level is estimated over 1000 repetitions. Data are generated using a Splines basis, while confidence bands are computed using the Fourier (top) and Legendre (bottom) basis families. The rows correspond to different model selection criteria and dimensions L, and the columns to various combinations of sample sizes (n,N).

L	n=40, N=25	n=150, N=25
L tilde	0.098	0.117
L.CV	0.090	0.084

L	n=40, N=25	n=150, N=25
L tilde	0.942	0.950
L.CV	0.588	0.593

529 The Fourier basis does not give a correct rate. On the other hand, the Legendre basis gives very
 530 satisfactory coverage rates for $L > 11$.

531 Next, we illustrate the \tilde{L} dimension selection method and compare it to the cross-validation method.
 532 Table 5 presents the coverage rates of the corresponding confidence bands estimated with the Fourier
 533 and Legendre basis, in the case $N = 25$ and $n \in \{40, 150\}$. Once again, we see that the Fourier
 534 basis does not give good results, either by cross-validation or by \tilde{L} . On the other hand, with the
 535 Legendre basis, the \tilde{L} method gives a satisfactory coverage rate, even if it is underestimated, whereas
 536 the cross-validation method is very poor. Moreover, the widths of the confidence bands selected
 537 with \tilde{L} and by cross validation are represented by boxplot in Figure 8. It can be seen that the cross-
 538 validation approach provides wider bands, even though their confidence level is not guaranteed. The
 539 method proposed in this paper provides a narrower band with a correct level of confidence. We thus
 540 recommend to use the Legendre family with the criteria \tilde{L} .

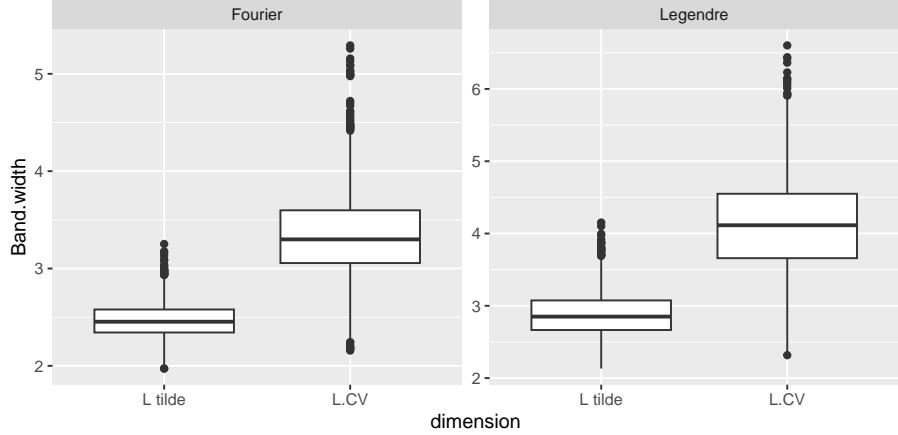


Figure 8: Width of confidence bands with model selection under model misspecification. The average width of the confidence bands is evaluated over 1000 repetitions. Data are generated using a Splines basis, while bands are computed with the Fourier (top) and Legendre (bottom) basis families. Rows correspond to combinations of model selection criteria and dimensions L , and columns to different sample size pairs (n, N).

541 7 Real data analysis

542 In this section, we illustrate the proposed method on the Berkeley Growth Study data. It consists of
 543 the heights in centimeters of 39 boys at 31 ages from 1 to 18. We approximate these curves by the 3
 544 basis Legendre, Splines and Fourier. We select the level of each basis using the method introduced in
 545 Section 5.

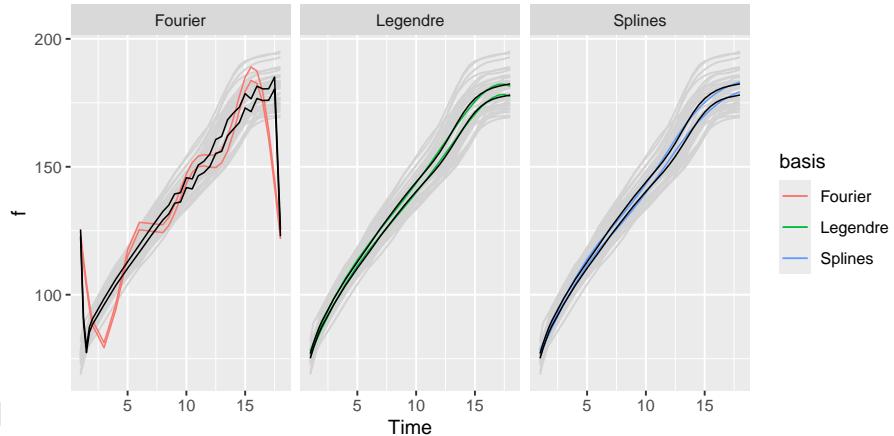


Figure 9: Real data analysis example. We display the confidence bands for Fourier (left), Legendre (middle) and Splines (right) basis on the Berkeley Growth Study data. Black curves correspond to the confidence bands with L_{max} , while colored one are the confidence bands with $L \tilde{t}$.

546 In Figure 9, we display the confidence bands associated with Section 3 in black and those associated
 547 with Section 5, for the three basis. As the data is not periodic, the Fourier basis is meaningless, as is
 548 the associated confidence band, whatever the dimension considered. Splines and Legendre basis give
 549 similar confidence bands. Analyzing the width of the bands in Table 6, compared to that obtained
 550 with L_{max} , we find that they are less smooth but also smaller, and from our empirical study we guess
 551 that it makes a trade-off between bias and variance.

Table 6: Real data analysis example, Berkeley Growth Study data. We display the width of the confidence bands for Fourier, Legendre and Splines basis for the confidence band of Section 3 with Lmax and the confidence band of Section 5. We also precise the dimension of the selected model.

	Basis		
	Legendre	Splines	Fourier
Width Lmax	2.12	2.12	2.20
Width selected	1.99	1.95	2.08
Model selected	6.00	5.00	7.00

552 8 Conclusion

553 This paper discusses the construction of confidence bands when considering a functional model.
 554 Depending on the nature of the family (an orthogonal or orthonormal basis, or simply a vector space),
 555 the theoretical guarantees of the linear estimator are recalled and illustrated. Several confidence
 556 bands are then proposed. An extensive experimental study on Fourier, Legendre, and Spline basis
 557 illustrates the theoretical and methodological propositions, and a real data study is proposed to
 558 conclude the paper.

559 First, when considering a functional family with fixed dimension, we discuss the confidence band
 560 derived from Sun and Loader (1994). It is biased if the dimension is not high enough to approximate
 561 well the true function. We then propose a new confidence band that corrects this bias. To do this,
 562 the bias is estimated and the additional randomness is controlled. A selection criterion is proposed
 563 to select the best dimension. Unfortunately, the two types of randomness lead to a wider confidence
 564 band, and this result is therefore no more interesting than the naive one, which consists of taking
 565 the largest possible dimension L_{\max} . Finally, a heuristic selection criterion is proposed to select the
 566 dimension on the first confidence band, which has not corrected the bias. It takes into account the
 567 bias as well as the variance, to select a moderate dimension. Numerical experiments show that this
 568 criterion, combined with the Legendre basis, achieves the best performance when considering the
 569 confidence level and the width of the corresponding simultaneous confidence band.

570 An interesting next step, but out of the scope of this paper, is a theoretical study of this criterion.
 571 No result, to our knowledge, exists for confidence bands with the supremum norm. The Euclidean
 572 norm has been extensively studied, but is not of interest here, where we want to ensure that the
 573 tube is valid as a whole. The supremum norm, on the other hand, is difficult to study theoretically.
 574 Furthermore, a key point here is the randomness of the criterion, which must also be taken into
 575 account, through an oracle inequality for example.

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636 9 Appendix: proofs

637 9.1 Proof of Proposition 2.1

638 Let us prove the first point. We have

$$\mathbb{E}(\hat{\mu}^L) = (\mathbf{B}_L^T \mathbf{B}_L)^{-1} \mathbf{B}_L^T \mathbb{E}(\mathbf{y}) = (\mathbf{B}_L^T \mathbf{B}_L)^{-1} \mathbf{B}_L^T \mathbf{B}_{L^*} \mu^{L^*} =: \underline{\mu}^L.$$

639 The theory of the linear model gives that the variance of $\underline{\mu}^L$ is equal to $\sigma^2 (\mathbf{B}^T \mathbf{B})^{-1} \mathbf{B}^T \Sigma \mathbf{B} (\mathbf{B}^T \mathbf{B})^{-1}$ with
640 $\Sigma = \text{Diag}(\Sigma_1, \dots, \Sigma_N)$ the $nN \times nN$ covariance matrix of \mathbf{y} . So finally, we have

$$\hat{\mu}^L \sim \mathcal{N}(\underline{\mu}^L, \sigma^2 \Sigma_B^{L,L^*}).$$

641 Now we can easily deduce the distribution of $\underline{f}^L(t)$, for each $t \in [0, 1]$:

$$\underline{f}^L(t) - \mathbf{f}^L(t) \sim \mathcal{N}(0, \sigma^2 B(t) \Sigma_B^{L,L^*} B(t)^T).$$

642 To prove that $(\hat{f}^L - f^L)$ is a Gaussian process, we consider any finite sequence of times $(t_1, \dots, t_d) \in$
643 $[0, 1]$. The sequence $(\hat{f}^L(t_1) - f^L(t_1), \dots, \hat{f}^L(t_d) - f^L(t_d))$ is Gaussian, centered, and the covariance is
644 equal to $\text{cov}(\hat{f}^L(t_1) - f^L(t_1), \hat{f}^L(t_2) - f^L(t_2)) = \sigma^2 B(t_1) \Sigma_B^{L,L^*} B(t_2)^T$. Thus, the process is Gaussian.

645 9.2 Proof of Theorem 3.2

646 For all t , for all $\omega \in \Omega$,

$$\lim_{n \rightarrow +\infty} \underline{f}_n^L(t) - f^L(t) = 0$$

647 which means for all $\varepsilon > 0$, there exists N_0 such that for all $n > N_0$,

$$|\underline{f}_n^L(t) - f^L(t)| \leq \varepsilon.$$

648 Then, we have, with probability $1 - \alpha$,

$$|\underline{f}^L(t) - \underline{f}_n^L(t)| + |\underline{f}_n^L(t) - f^L(t)| \leq \hat{d}^L(t) + \varepsilon$$

649 with $\hat{d}^L(t) = \hat{c}^L \sqrt{\hat{C}_L(t,t)/N}$ and \hat{c}^L defined as the solution of Equation 4.

650 Then, with probability larger than $1 - \alpha$,

$$|\hat{f}^L(t) - \underline{f}_n^L(t) + \underline{f}_n^L(t) - f^L(t)| \leq \hat{d}^L(t) + \varepsilon$$

651 9.3 Proof of Proposition 4.1

652 To simplify the notations, let us denote $a(t) = \underline{f}^L(t) - \underline{f}_1^L(t)$ and $b(t) = \underline{f}^{L_{\max}, L^*}(t) - \underline{f}^L(t) - (\underline{f}_2^{L_{\max}, L^*}(t) -$
653 $\underline{f}_2^L(t))$. We have

$$\begin{aligned} P(\exists t |a(t) + b(t)| \geq \hat{d}_1^L(t) + \hat{d}_2^{L_{\max}}(t)) &\leq P(\exists t |a(t)| + |b(t)| \geq \hat{d}_1^L(t) + \hat{d}_2^{L_{\max}}(t)) \\ &= P(\exists t |a(t)| \geq \hat{d}_1^L(t)) P(\exists t |b(t)| \geq \hat{d}_2^{L_{\max}}(t)) = \alpha \beta. \end{aligned}$$

654 The last equality holds thanks to the independence of the two sub-samples.

655 10 Appendix: more experiments

656 The properties of the coefficients are illustrated in Figure 10. The true dimension is $L^* = 11$. Three
 657 families are considered, Fourier, Legendre and Splines. The plots display the absolute difference
 658 between the coefficients $\mu_\ell^{L^*}$ and the projected coefficients μ_ℓ^L , for different ℓ in x-axis and for different
 659 values of L and n in the y-axis, namely a case with $L < L^*$ and two values of n : $L = 7, n = 20$ and
 660 $L = 7, n = 100$; and a case with $L > L^*$ and two values of n : $L = 15, n = 20$ and $L = 15, n = 100$.
 661 The absolute difference is represented as a gradient of color, this gradient being adapted to each
 662 functional family. We can see that as Legendre (resp. Fourier) are orthonormal (resp. orthogonal)
 663 families, the differences are close to 0 when $L = 15$, whatever the values of n . When $L < L^*$, the
 664 difference is close to 0 when n is large. This property does not hold for the spline family, which is
 665 not orthogonal.

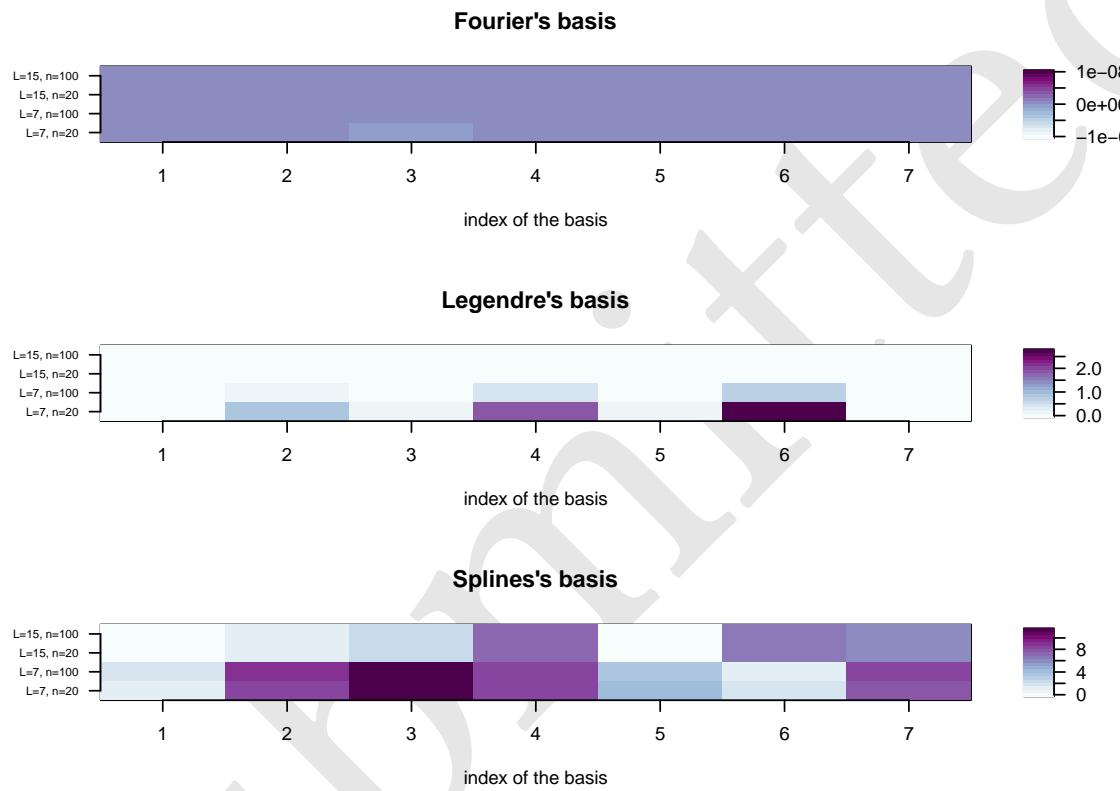


Figure 10: Illustrative example. The true dimension is 11, we generate the coefficients with three families, Fourier (which is orthogonal), Legendre (which is orthonormal) and the splines (which are not orthogonal wrt the standard scalar product). In the y-axis, two dimensions of the family (7 or 15) and two numbers of timepoints (20 or 100) are compared. We plot in x-axis the value of the absolute difference between the true coefficients and their approximations for the first 7 coefficients of the basis. The color scale is adapted to each functional basis.