

From multiple Gaussian sequences to functional data and beyond: a Stein estimation approach

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Summary. We expand the notion of Gaussian sequence models to n experiments and propose a Stein estimation strategy which relies on pooling information across experiments. An oracle

in the limit $m \rightarrow \infty$. This follows from Le Cam equivalence between expression (2) and the white noise model

$$Y(dt) = f(t) dt + \sigma m^{-1/2} W(dt), \quad t \in [0, 1], \quad (3)$$

W being standard Brownian motion. This connection has been studied by Brown and Low (1996), Brown *et al.* (2002) and Reiß (2008), among others. The white noise model (3) acts on an orthonormal basis $\{\psi_k\}_{k \in \mathbb{N}}$ of $L^2[0, 1]$ to give rise to the GSM (1) with $\theta_k = \langle f, \psi_k \rangle$. For any estimator \hat{f} of f , isometry leads to $\mathbb{E} \|f - \hat{f}\|_{L_2}^2 = \sum_{k=1}^{\infty} \mathbb{E}(\theta_k - \hat{\theta}_k)^2$, where $\hat{\theta}_k = \langle \hat{f}, \psi_k \rangle$. This reduces the problem of estimating f under L^2 -loss to the problem of estimating a sequence of normal means $\theta = (\theta_k)_{k \in \mathbb{N}}$ under l_2 -loss. The appeal of this framework is that a function of practical interest often has a natural characterization in terms of geometric constraints on its (generalized) Fourier coefficients θ_k in a suitable basis, and may be grouped into a collection \mathcal{F} of possible generating mechanisms for expression (2). By distilling the central issues at play, reduction to expression (1) has inspired many estimation procedures with adaptivity properties. See Donoho (1993), Donoho *et al.* (1995), Cai (1999), Cavalier and Tsybakov (2002) and Zhang (2005) for original work in this direction and Candes (2006), Cai (2012) and Johnstone (2015) for comprehensive overviews. This framework has also facilitated understanding of frequentist and Bayesian properties of simple Bayesian non-parametric models. See Freedman (1999), Zhao (2000), Belitser and Ghosal (2003) and Szabó *et al.* (2013) for studies in this direction.

Modern scientific experiments are often conducted simultaneously with data sampled from multiple ‘similar’ functions, such as images and voice signals, which motivates grouping GSMs corresponding to individual experiments. In this paper, we expand on the notion of GSM (1) to study recovery of multiple sequences, namely the multiple GSMs of size n ,

$$Y_{ik} = \theta_{ik} + \sigma m^{-1/2} z_{ik}, \quad k \in \mathbb{N}, \quad i = 1, \dots, n, \quad (4)$$

where $z_{ik} \sim^{\text{IID}} N(0, 1)$. This can be viewed as an idealization of observing n non-parametric experiments,

$$y_{ij} = f_i(x_{ij}) + \sigma z_{ij}, \quad x_{ij} \in [0, 1], \quad i = 1, \dots, n, \quad j = 1, \dots, m, \quad (5)$$

corresponding to the central model of functional data analysis (FDA) which has attracted considerable interest in recent decades. See Ramsay and Silverman (2005) for an introduction and examples.

The main contributions of this paper are twofold. The first part focuses on simultaneous recovery of the effects $\{\theta_i\}_{i \leq n}$, where $\theta_i = (\theta_{ik})_{k \in \mathbb{N}}$, from multiple GSMs (4). A form of Stein estimation, based on information pooling across experiments, is proposed and its properties are derived with the aid of new concentration results. The method is shown to attain the optimal rate for recovery of n experiments in a uniform manner and enjoys a robustness guarantee in a minimax sense. Moreover, the theoretical analysis suggests an explicit tuning-free form which governs the amount of shrinkage parsimoniously under a general condition $m^{\gamma_1} \lesssim n \lesssim m^{\gamma_2} \rightarrow \infty$, for any $\gamma_2 \geq \gamma_1 >$

and random design, which covers standard cases that are considered in the functional data literature (Hall *et al.*, 2006; Cai and Yuan, 2011). We further show that the theoretical guarantees of the recovery proposed continue to hold for bases on which the projected coefficients exhibit decaying correlations, and we present concrete examples of process–basis pairs satisfying such assumptions. Although useful in many areas, common FDA methods based on non-parametric smoothing suffer from some drawbacks. Chief among these are complicated theoretical properties and reliance on computationally expensive procedures. Hence a key motivation for studying multiple GSMs (4) is to provide a simplified but foundational framework for functional data which might encourage development of new methods with properties that are both easy to establish and relate transparently to other areas of statistics. On the computational side, the method operates in $O\{nm \log(m)\}$ time, in contrast with standard smoothing-based FDA techniques that typically operate in at least $O(nm^2 + m^3)$ time (Ramsay and Silverman, 2005; Yao *et al.*, 2005). This implies potentially significant computational savings and scalability to data of large dimensions or sizes. Further, our procedure may be employed in an on-line algorithm fashion: a new curve comes in, a transform is performed and threshold weights are updated, which makes our method potentially useful in the context of realtime data collection and processing.

The rest of the paper is organized as follows. In Section 2 we draw inspiration from an oracle strategy known to achieve optimal recovery rates under the conditional l_2 -risk metric. Risks of the proposed Stein estimation are related to those of the oracle strategy via a set of concentration inequalities on the conditional measures. This leads to a theory of simultaneous recovery which gives a precise account of the shrinkage and extends seamlessly to the case of unknown variance. In Section 3, we make the connection to the functional data model (4) through Le Cam asymptotic equivalence and extrapolate our recovery theory to more general correlation settings that one might encounter in practice. In Section 4, we first present a simulation study to support the recovery method and its theoretical properties in the setting of multiple GSMs; then we demonstrate its performance and computational gains by using the phoneme data set (Hastie *et al.*, 1995). The computer code and data for reproducing the results are available from <http://www.utstat.utoronto.ca/fyao/GSM-FDA-code.zip>. We conclude in Section 5 with discussion on potential application to other statistical problems that may deserve further investigation, such as multiple-change-point detection for penal data. For brevity, we collect proofs of all theoretical results and some additional simulation results in the on-line supplementary material.

2. Multiple Gaussian sequences and Stein estimation

2.1. Problem setting and objective

Before moving forwards, we outline some notation that is used throughout. For a function $f: \mathcal{D} \rightarrow \mathbb{R}$, mapping some domain \mathcal{D} into \mathbb{R} , we let $\text{supp}(f)$ denote the support of f , i.e. $\text{supp}(f) = \{x \in \mathcal{D} : f(x) \neq 0\}$. We let ‘ \perp ’ denote statistical independence, $(x)_+ = \max(0, x)$ for $x \in \mathbb{R}$ and, for $x \in \mathbb{R}^m$ with positive components, we let $x_{(j)}$ denote the non-increasing order statistics of the co-ordinates, such that $x_{(1)} \geq x_{(2)} \geq \dots \geq x_{(m)}$. For n

across i for given k . A common model in the non-parametric literature on GSMs (1) takes $\lambda_k^{-1/2}\theta_k \sim \text{IID } N(0, 1)$ independent of z_k , with $\lambda_k = 2\alpha k^{-(2\alpha+1)}$ and $\alpha > 0$. We use this as our model for GSMs (4), with $\theta_{1k}, \dots, \theta_{nk} \sim \text{IID } \theta_k$ independent of the z_{ik} , but relax the variance decay to

$$\begin{aligned} \lambda_{(k)} &\propto k^{-(2\alpha+1)}, & k \leq m, \\ \lambda_k &\propto k^{-(2\alpha+1)}, & k > m. \end{aligned} \quad (6)$$

Thus the bulk of each signal is contained in the first m co-ordinates, but the location and ordering of sizable effects are unknown *a priori*. We give a graphical demonstration in Section 4.1 showing that this relaxation is suitable for modelling functions with striking local features from a smoothness perspective in a similar manner to wavelet estimation in non-parametric regression (Donoho and Johnstone, 1994). In what follows, we let $\mathbf{E}_i(\cdot) = \mathbf{E}_{\theta_i}(\cdot) = \mathbf{E}(\cdot | \theta_i)$ denote expectation conditional on the i th effect.

Remark 1. The regularity setting (6) can be regarded as randomization of weak l_p decay conditions (up to m) with their origin in Donoho (1993) who noted that they are closely related to Besov smoothness in the context of wavelet coefficients. Standard properties of Gaussian variables lead to

$$\max_k k^{1/p} |\theta|_{(k)} \lesssim \max_k k^{1/p-(\alpha+1/2)} \log(1+k)^{1/2},$$

and so we are in every weak l_p -space for $p > 2/(2\alpha + 1)$, with $|\theta_k|/\log(1+k)^{1/2}$ lying in $p = 1/(2\alpha + 1)$, where a rigorous argument is given in the on-line supplementary material. These spaces are known to form important generalizations of the traditional Hölder and Sobolev type of smoothness spaces. As discussed in Donoho (1993) and Candes (2006), once a suitable basis has been specified, such decay conditions set the frontier of statistical recovery at non-linear approximation spaces.

Remark 2. We assume a centred model (5) for functional data that corresponds to mean 0 GSMs (4), as research in FDA mostly focuses on characterizing random realizations and covariance structure of an underlying process. Estimation of the mean function is usually considered an easier task by standard means of non-parametric regression, such as kernel type (Yao *et al.*, 2005; Li and Hsing, 2010) or spline type (Ramsay and Silverman, 2005) smoothing which attains a univariate convergence rate that is asymptotically negligible relative to simultaneous recovery or covariance estimation. Hence the methodology proposed can be applied by subtracting the estimated mean function (or simply the cross-sectional mean when observed on a common grid).

We now relate simultaneous recovery of $\theta_i = (\theta_{ik})_{k \in \mathbb{N}}$, for $i = 1, \dots, n$, to an oracle framework. Let $\mathbf{E}(\cdot | \theta_i) = \mathbf{E}_{\theta_i}(\cdot) = \mathbf{E}_i(\cdot)$ denote conditional expectation and define the conditional l_2 -risk of an estimator $\hat{\theta}_i$ by

$$\mathcal{R}_{i,m}(\hat{\theta}_i) \triangleq \mathbf{E}_i \|\theta_i - \hat{\theta}_i\|_{l_2}^2. \quad (7)$$

Our goal is to devise an estimation strategy $\{\hat{\theta}_i\}_{i \leq n}$ that is faithful to the effects $\{\theta$

a factor of the optimal average risk attained by the linear oracle $\hat{\theta}_{ik}^{o,a} = \lambda_k Y_{ik} / (\lambda_k + \sigma^2/m)$, i.e. $\mathbf{E} \|\theta_i - \hat{\theta}_i^{o,a}\|_{l_2}^2 = \sum_{k=1}^{\infty} (\lambda_k/m) / (\lambda_k + 1/m) \propto m^{-2\alpha/(2\alpha+1)}$. We show in Section 2.3 that the conditional risks of this linear oracle, $\mathcal{R}_{i,m}^* = \mathbf{E}_i \|\theta_i - \hat{\theta}_i^{o,a}\|_{l_2}^2$, can be controlled uniformly near its average. From this perspective, no procedure can do significantly better than $\hat{\theta}_{ik}^{o,a}$ which is rate optimal among diagonal linear rules. Further, these rules are known to perform within a small factor of the minimax optimal estimators over a broad range of parameter spaces (Donoho *et al.*, 1990). Such considerations motivate the search for recovery strategy $\hat{\theta}_i$ performing as well as the average case oracle $\hat{\theta}_i^{o,a}$.

2.2. Stein estimation motivated by conditional concentration

The main idea guiding this paper is that models that are generated by similar experiments put us in an empirical-Bayes-type setting where information pooling improves estimation. In this setting, concentration of measure can be used to guide design of estimators and to quantify how information pooling improves estimation measured by risks conditioned on the effects. For the moment we take $\sigma^2 = 1$, treating the case of unknown variance in Section 2.6. Note that the average case oracle $\hat{\theta}_{ik}^{o,a}$ can be written equivalently as $\hat{\theta}_{ik}^{o,a} = [1 - (n/m) / \{n(\lambda_k + 1/m)\}]_+ Y_{ik}$. Thus, when the relative error that is incurred in approximating $n(\lambda_k + \sigma^2/m)$ by $\|Y_{\cdot k}\|^2$ is sufficiently small, it is natural to consider standard (positive part) Stein estimation

$$\hat{\theta}_{ik}^S = \begin{cases} \beta_{mn,k} Y_{ik}, & k \leq m \\ 0, & k > m \end{cases} \quad \beta_{mn,k} = \left(1 - \frac{n/m}{\|Y_{\cdot k}\|^2}\right)_+. \quad (8)$$

Similar ideas have been employed in the non-parametric setting (2) by Cai (1999), Cavalier and Tsybakov (2002) and Zhang (2005) from different perspectives.

In this and the next subsection, we explore the intuition and theory to arrive at the proposed Stein estimation strategy that is different from expression (8),

$$\hat{\theta}_{ik}^{RS} = \begin{cases} \alpha_{mn,k} Y_{ik}, & k \leq m \\ 0, & k > m \end{cases} \quad \alpha_{mn,k} = \left\{1 - [1 + 2\sqrt{\{12 \log(m)/n\}}] \frac{n/m}{\|Y_{\cdot k}\|^2}\right\}_+. \quad (9)$$

We begin with a new concentration of measure result, conditional on the effects, which is used to assess the relative error of approximating $n(\lambda_k + \sigma^2/m)$ by $\|Y_{\cdot k}\|^2$; see the on-line supplementary material for its proof. For $\delta \in (0, 1)$, we consider collections of arrays whose components satisfy norm constraints indexed by δ . Specifically, given $\lambda_1, \dots, \lambda_m$, define the sets $A_{k,\delta}$, $k = 1, \dots, m$, and A_δ^m by complement as follows:

$$A_{k,\delta}^c = \{(1 - \delta)n(\lambda_k + 1/m) \leq \|Y_{\cdot k}\|^2 \leq (1 + \delta)n(\lambda_k + 1/m)\} \quad (10)$$

and set $A_\delta^{m,c} = \cap_{k \leq m} A_{k,\delta}^c$. Denote $\lambda = (\lambda_1, \lambda_2, \dots)$ and $\mathbf{P}_i(\cdot) = \mathbf{P}(\cdot | \theta_i)$.

Lemma 1. Consider multiple GSMs (4) with the decay assumption (6), for all $\delta \in (0, \frac{1}{2})$ and $i = 1, \dots, n$: we have

$$\mathbf{P}_i(A_{k,\delta}) \leq 3 \exp(\delta \|\theta_i^2 / \lambda\|_{m,\infty}) \exp(-n\delta^2/6), \quad (11)$$

$$\mathbf{P}_i(A_\delta^m) \leq 3 \exp(\delta \|\theta_i^2 / \lambda\|_{m,\infty}) \exp\{-n\delta^2/6 + \log(m)\}. \quad (12)$$

This result inspires different Stein estimates (8) and sets the stage for bounding the conditional risks of the estimator proposed. Intuitively, for ‘most’ effects, it is seen that $\|\theta_i^2 / \lambda\|_{m,\infty}^2 \approx 2 \log(m)$. Thus, if $m^{\gamma_1} \lesssim n \lesssim m^{\gamma_2}$ for any $\gamma_2 \geq \gamma_1 > 0$, taking $\delta^2 = C \log(m)/n$ with $C > 6$ guarantees that the conditional probabilities in inequality (12) are small while $\delta \rightarrow 0$ as $m, n \rightarrow \infty$.

To understand the behaviour of the traditional Stein estimate (8) in multiple GSMs, note that $\|Y_{\cdot k}\|^2 \sim (\lambda_k + 1/m)\chi^2(n)$ with $\mathbf{E}\|Y_{\cdot k}\|^2 = n(\lambda_k + 1/m)$. Since $\lambda_k \propto k^{-(2\alpha+1)}$ tends to 0 quickly, once $k > m^{1/(2\alpha+1)}$ the signals decay rapidly below the noise level and in this range $\|Y_{\cdot k}\|^2 \approx \chi^2(n)/m$. On the basis of this intuition, we expect approximately half of the $\{\|Y_{\cdot k}\|^2\}_{k \leq m}$ to exceed n/m with corresponding standard Stein weights $\beta_{mn,k} > 0$. However, given the fast decay of λ_k , we expect that only of the order of $m^{1/(2\alpha+1)}$ of the $\{Y_{ik}\}_{k \leq m}$ contain sizable signals, whereas the rest mainly contain noise. Further, when the norms fluctuate within the regime of high probability and $\lambda_k \ll 1/m$, many of the $\|Y_{\cdot k}\|^2 \approx (1 + \delta)n(\lambda_k + 1/m)$, with $\delta = \sqrt{\{C \log(m)/n\}}$. This gives

$$\left| \beta_{mn,k} - \frac{\lambda_k}{\lambda_k + 1/m} \right| / \frac{\lambda_k}{\lambda_k + 1/m} \approx \frac{\delta}{m\lambda_k},$$

which can be arbitrarily large because of the rapid decay of λ_k . In other words, we do better by forcing most $\beta_{mn,k}$ to 0 to mimic the oracle weights in the range $\lambda_k \ll 1/m$.

This motivates a different Stein threshold in expression (8). Note that, on the event $A_\delta^{m,c}$, we have $\|Y_{\cdot k}\|^2 \leq (1 + \delta)n(\lambda_k + 1/m)$. Thus for $\lambda_k \ll 1/m$, i.e. $k \gg m^{1/(2\alpha+1)}$, we expect that $\|Y_{\cdot k}\|^2 \lesssim (1 + \delta)n/m < (1 + 2\delta)n/m$. In the light of this, we propose to lift the threshold level to $(1 + 2\delta)n/m$ to force most weights in this range to 0, which leads to the new Stein weights $\alpha_{mn,k} = [1 - \{(1 + 2\delta)n/m\} / \|Y_{\cdot k}\|^2]_+$ for $k \leq m$. The effect of δ on estimation quality is precisely quantified in an extended version of theorem 2, presented in the on-line supplementary material, which suggests the explicit form (9). Since lemma 1 guarantees that, conditionally on the effects θ_i , the events $A_\delta^{m,c}$ encompass most of the probability space with the right choice of $\delta \rightarrow 0$, we expect that the strategy proposed retains only important signals and forces the rest to zero, leading to desired model parsimony.

2.3. Adaptive conditional risks of simultaneous recovery

On the basis of lemma 1 we can derive a new oracle inequality that relates the componentwise conditional risks of the Stein estimates $\hat{\theta}_{ik}^{\text{RS}}$ to those attainable by the oracle strategy $\hat{\theta}_{ik}^{o,a}$. The derivation is given in the on-line supplementary material, employing techniques of technical interest for assessing Stein or other shrinkage estimates in similar settings. Denote the componentwise conditional risks of the oracle strategy $\hat{\theta}_{ik}^{o,a}$ by $\mathcal{R}_{i,m}^*(k) = \Delta \mathbf{E}_i(\theta_{ik} - \hat{\theta}_{ik}^{o,a})^2$, where simple calculation yields

$$\mathcal{R}_{i,m}^*(k) = \frac{\lambda_k \sigma^2 / m}{\lambda_k + \sigma^2 / m} + \frac{\sigma^4 / m^2}{\lambda_k + \sigma^2 / m} (\theta_{ik}^2 - \lambda_k), \quad (13)$$

where $\sigma^2 = 1$ is written explicitly for generality, and isometry gives $\mathcal{R}_{i,m}^* = \sum_{k=1}^\infty \mathcal{R}_{i,m}^*(k)$. Similarly, for any estimator $\hat{\theta}_i$ denoting $\mathcal{R}_{i,m}(\hat{\theta}_i, k) = \mathbf{E}_i(\theta_{ik} - \hat{\theta}_{ik})^2$ gives $\mathcal{R}_{i,m}(\hat{\theta}_i) = \sum_{k=1}^\infty \mathcal{R}_{i,m}(\hat{\theta}_i, k)$.

Theorem 1. Consider multiple GSMs (4) with the decay assumption (6), for $i = 1, \dots, n$ and $k = 1, \dots, m$:

$$\mathbf{E}_i(\theta_{ik} - \hat{\theta}_{ik}^{\text{RS}})^2 = \mathcal{R}_{i,m}^*(k) + e_{ik}, \quad (14)$$

where $\mathcal{R}_{i,m}^*(k) = \mathbf{E}_i(\theta_{ik} - \hat{\theta}_{ik}^{o,a})^2$.

where $C_\delta = 3(6 + \delta)/(1 - \delta)$ and $C = \sqrt{24} + 4\sqrt{12}$ are bounded and $\mathbf{P}_i(A_\delta^m)$ satisfy the probability bounds in inequality (12).

This oracle inequality sets the theoretical basis for evaluating the conditional risks of simultaneously recovering the effects $\{\theta_i\}_{i \leq n}$. Note that the componentwise conditional oracle risks $\mathcal{R}_{i,m}^*(k)$ differ from the optimal average risk by random perturbations. When we sum these risks to obtain $\mathcal{R}_{i,m}^*$, the decay condition on λ_k (6) with concentration argument ensures that cancellations keep $\mathcal{R}_{i,m}^*$ of the same order of the average risk. For brevity we provide a condensed version of our theorem quantifying the maximal conditional risks, which shows that the proposed recovery strategy adapts to the average case oracle. An expanded version and its proof are given in the on-line supplementary material.

Theorem 2. Consider multiple GSMs (4) with the decay assumption (6), and suppose that $n, m \rightarrow \infty$ with $m^{\gamma_1} \lesssim n \lesssim m^{\gamma_2}$ for any $\gamma_2 \geq \gamma_1 > 0$. Then

$$\max_{i \leq n} \mathcal{R}_{i,m}^* = \{1 + o_{a.s.}(1)\} \sum_{k=1}^{\infty} \frac{\lambda_k/m}{\lambda_k + 1/m} \propto m^{-2\alpha/(2\alpha+1)}, \quad i = 1, \dots, n. \quad (16)$$

Further, the conditional risks $\mathcal{R}_{i,m}(\hat{\theta}_i^{\text{RS}}) = \mathbf{E}_i \|\theta_i - \hat{\theta}_i^{\text{RS}}\|_{l_2}^2$ adapt simultaneously to the oracle risks $\mathcal{R}_{i,m}^*$ for any choice of $\kappa \geq 2$ with $\delta = \sqrt{4(\kappa + 1) \log(m)/n} \rightarrow 0$:

$$\max_{i \leq n} \mathcal{R}_{i,m}(\hat{\theta}_i^{\text{RS}}) / \mathcal{R}_{i,m}^* = 1 + o_{a.s.}(1). \quad (17)$$

It follows from the expanded version of theorem 2 in the supplementary material that, without prior knowledge of the α governing decay of the $\{\lambda_k\}_{k \in \mathbb{N}}$, $\kappa = 2$ is the smallest value such that $\max_{i \leq n} e_i = o(m^{-2\alpha/(2\alpha+1)})$ almost surely, which yields an explicit form of the Stein estimates defined in expression (9).

2.4. Risk comparisons with individual blocking

To appreciate the advantages of information pooling by the method proposed, we compare with the risk performance of standard ‘pathwise’ blocking estimators that use the data from that individual only, in the context of multiple GSMs; see Tsybakov (2009) and Johnstone (2015) for details. To construct a pathwise blocking Stein estimate, given an increasing sequence of numbers in $[m] = \{1, \dots, m\}$, $1 \leq j_1 < j_2 < \dots < j_{K_m} = m$ with $K_m \rightarrow \infty$ and setting $j_0 = 0$, we form a partition of $[m]$ into blocks $\mathcal{B} = \{B_1, \dots, B_{K_m}\}$, where $B_k = \{j_{k-1} + 1, \dots, j_k\}$. Denote the cardinality of the k th block by $|B_k|$ and set $\mathbf{a}_{B_k} = (a_{j_{k-1}+1}, \dots, a_{j_k})^T$ for $\mathbf{a} \in \mathbb{R}^m$; one estimates the components of the k th block by Stein shrinkage,

$$\hat{\theta}_{i,B_k} = \left(1 - \frac{|B_k|/m}{\|\mathbf{Y}_{i,B_k}\|_2^2}\right)_+ \mathbf{Y}_{i,B_k}, \quad (18)$$

and correspondingly θ_i by $\hat{\theta}_i^{\mathcal{B}} = (\hat{\theta}_{i,B_1}, \dots, \hat{\theta}_{i,B_{K_m}}, 0, \dots)^T$, with the conditional risks denoted by $\mathcal{R}_i(\hat{\theta}_i^{\mathcal{B}}) = \Delta \mathbf{E}_{\theta_i} \|\theta_i - \hat{\theta}_i^{\mathcal{B}}\|_{l_2}^2$.

Theorem 3. Consider multiple GSMs (4) with the decay assumption (6), and suppose that $n, m \rightarrow \infty$ with $m^{\gamma_1} \lesssim n \lesssim m^{\gamma_2}$ for any $\gamma_2 \geq \gamma_1 > 0$. For any blocking scheme \mathcal{B} satisfying $K_m = o\{m^{1/(\alpha+1/2)} / \log(m)\}$ and containing at most $O\{\log(m)\}$ blocks of size less than $\log(m)$, the blocking estimator (18) cannot outperform the average case oracle. The lower bound of the conditional risks is given by

$$\min_{i \leq n} \mathcal{R}_i(\hat{\theta}_i^{\mathcal{B}}) \geq \{1 + o_{a.s.}(1)\} \sum_{k=1}^{\infty} \frac{\lambda_k/m}{\lambda_k + 1/m} \propto m^{-2\alpha/(2\alpha+1)}.$$

Further, in this setting, when $K_m = o\{m^{1/(2\alpha+1)} / \log(m)\}$ and $\alpha \geq \frac{1}{2}$, there are always permutations of $(\lambda_1, \dots, \lambda_m)^T$ under which $\hat{\theta}_i^{\mathcal{B}}$ performs poorly such that $\mathcal{R}_i(\hat{\theta}_i^{\mathcal{B}}) \gg m^{-2\alpha/(2\alpha+1)}$ with high probability for each $i = 1, \dots, n$.

Standard blocking schemes, such as dyadic and weak geometric systems, satisfy conditions in theorem 3 and have a fundamental limit at performance of the average case oracle. The crucial drawback of these blocking estimators is that they require knowledge of the decay ordering, as there must be some block of size at least $m^{2\alpha/(2\alpha+1)} \log(m)$. If a permutation places too many large effects in this block, then, with high probability, the realized effects will be larger than $|B|/m \gtrsim m^{-1/(2\alpha+1)} \log(m)$, resulting in a crude lower bound $m^{-1/(2\alpha+1)} \log(m) \gg m^{-2\alpha/(2\alpha+1)}$. This provides rationale for not pooling across indices k in this setting (e.g. Cai (1999) and Zhang (2005)), because performance of these strategies relies on coefficients in a given block being of similar size, which generally requires an implicit assumption on the decay. Although pooling over k would alleviate the condition $n \gtrsim m^{\gamma_1}$ in the case of standard decay, $\lambda_k \propto k^{-(2\alpha+1)}$, in the more general setting $\lambda_{(k)} \propto k^{-(2\alpha+1)}$ such strategies can be highly suboptimal. Nevertheless, it remains an open question whether pooling over the experiments $i = 1, \dots, n$ is strictly necessary, which deserves further investigation.

2.5. Robustness guarantee in minimax sense

To provide a robustness guarantee for the Stein estimates (9) in a minimax sense, we specify a sequence of parameter spaces which account for the increasing number of experiments that we need to control. When we restrict to the first m coefficients of the $\{\theta_i\}_{i \leq n}$, it is reasonable to expect that these decay at the order of $\sqrt{\{\lambda_k \log(mn)\}}$, which suggests the scaling of the spaces. Thus we fix $a, b > 0$ and define

$$A_{mn,k}(\lambda_k) = \{x \in l_2 : x_k^2/\lambda_k \leq a \log(mn)\}, \quad B_{mn,k}(\lambda_k) = \{x \in l_2 : x_k^2/\lambda_k \leq b \log(nk)\},$$

$$A_{mn}(\lambda) = \bigcap_{k \leq m} A_{mn,k}(\lambda_k), \quad B_{mn}(\lambda) = \bigcap_{k > m} B_{mn,k}(\lambda_k), \quad \Theta_{mn}(\lambda) = A_{mn}(\lambda) \cap B_{mn}(\lambda).$$

Then, with proper choices of a and b , one can guarantee that eventually all the θ_{ik} lie in $\Theta_{mn}(\lambda)$ and this becomes void if we substantially shrink the space. As a benchmark, we calculate the classical minimax risk,

$$\mathcal{R}_m\{\Theta_{mn}(\lambda)\} \propto m^{-2\alpha/(2\alpha+1)} \log(mn)^{1/(2\alpha+1)},$$

which follows from the fact that the $\Theta_{mn}(\lambda)$ are hyperrectangles and the bounds for minimax rates over these geometric regions given by Donoho *et al.* (1990). Theorem 2 indicates that our estimation strategy recovers the ‘within-sample’ signals θ_i simultaneously below the minimax risk over a sequence of parameter spaces which ‘just’ contains them. In the next theorem, we quantify the probabilistic assertion $\{\theta_i\}_{i \leq n} \subseteq \Theta_{mn}(\lambda)$ and provide a robustness guarantee to deviations from the distributional assumption in the following minimax sense. Suppose that we are given a fixed $\theta^* \in \Theta_{mn}(\lambda)$ and noisy observations on θ^* corresponding to model (1):

$$Y_k^* = \theta_k^* + m^{-1/2} z_k^*, \quad k \in \mathbb{N},$$

independent of $\{Y_{ik}\}_{i \leq n}$. Then we may construct an estimate $\hat{\theta}^{*RS}$ by using the weights $\alpha_{mn,k}$ (9) calculated from $\{Y_{ik}\}_{i \leq n}$ via $\hat{\theta}_k^{*RS} = \alpha_{mn,k} Y_k^*$. The following theorem asserts that the largest

risk that we incur by this procedure comes within a logarithmic factor of the minimax risk over $\Theta_{mn}(\lambda)$.

Theorem 4. Consider multiple GSMs (4) with the decay assumption (6), and suppose that $n, m \rightarrow \infty$ with $m^{\gamma_1} \lesssim n \lesssim m^{\gamma_2}$ for any $\gamma_2 \geq \gamma_1 > 0$.

- (a) It holds that $\max_{i \leq n} \|\theta_i^2/\lambda\|_{m,\infty} = \{1 + o_{a.s.}(1)\} \times 2 \log(nm)$; thus, if $a < 2$, eventually some $\theta_i \notin \Theta_{mn}(\lambda)$. Further, for any $a > (\gamma_1 + 2)/(\gamma_1 + 1)$ and $b > (2\gamma_1 + 3)/(\gamma_1 + 1)$, we have $\theta_1, \dots, \theta_n \notin \Theta_{mn}(\lambda)$ only finitely often.
- (b) Let $\hat{\theta}^{*RS}$ denote the procedure that was outlined above, and $\mathcal{R}_m(\hat{\theta}^{*RS}) = \mathbf{E}_{\theta^*} \|\theta^* - \hat{\theta}^{*RS}\|_2^2$ for any θ^* . Then we have

$$\sup_{\theta^* \in \Theta_{mn}(\lambda)} \mathcal{R}_m(\hat{\theta}^{*RS}) \propto \log(mn)^{2\alpha/(2\alpha+1)} \mathcal{R}_m\{\Theta_{mn}(\lambda)\}.$$

By coupling the arguments in the proofs of theorem 2 and theorem 4 in the on-line supplementary material, we also see that, if $\{\theta_{n+1}, \dots, \theta_{n+N}\}$ are independent draws from the same GSM (4) with $m^{\gamma_1} \lesssim N \lesssim m^{\gamma_2}$, owing to information pooling over $\{\theta_1, \dots, \theta_n\}$, we have, almost surely,

$$\max_{j \leq N} \mathbf{E}_{\theta_{n+j}} \|\theta_{n+j} - \hat{\theta}_{n+j}^{RS}\|_2^2 \propto m^{-2\alpha/(2\alpha+1)} = o[\mathcal{R}_m\{\Theta_{mn}(\lambda)\}],$$

where $\hat{\theta}_{n+j}^{RS}$ are obtained by applying $\alpha_{mn,k}$ (9) calculated from $\{Y_{ik}\}_{i \leq n}$ to the noisy sequence $\{Y_{n+j,k}\}_{k \leq m}$ via $\hat{\theta}_{n+j,k}^{RS} = \alpha_{mn,k} Y_{n+j,k}$. Moreover, part (a) in theorem 4 applies to various weakly dependent variables (e.g. Pickands (1969)) and part (b) holds regardless of dependence structures, which can be seen from its proof.

2.6. The case of unknown variance

We now consider the case of unknown variance σ^2 in multiple GSMs:

$$Y_{ik} = \theta_{ik} + \sigma m^{-1/2} z_{ik}, \quad i = 1, \dots, n, \quad k \in \mathbb{N},$$

with the goal of maintaining the risk properties of the proposed Stein estimates while using a data-based estimator $\hat{\sigma}^2$. Variance estimation has been extensively studied in non-parametric regression (2), mostly based on localized squared residuals (Hall and Carroll, 1989; Hall and Marron, 1990; Fan and Yao, 1998) or difference sequences (Müller and Stadtmüller, 1987; Hall *et al.*, 1990; Brown and Levine, 2007), among many others. It is rarely discussed in the GSM (1) which mainly serves as a theoretical device to study non-parametric regression problems. A relevant case is robust estimation using the median of the finest scale coefficients in a wavelet-transformed model (Donoho and Johnstone, 1994). In the multiple GSMs model (4), we propose a natural means of estimating σ^2 , based on concentration of measure.

Derivation of the key oracle inequality of theorem 1 relies on the sets $A_{k,\delta}^c$ containing most of the probability mass. In the case of unknown variance, the definitions extend to

$$A_{k,\delta}^c = \{(1 - \delta)(\lambda_k + \sigma^2/m) \leq \|Y_{\cdot k}\|^2/n \leq (1 + \delta)(\lambda_k + \sigma^2/m)\},$$

and $A_\delta^{m,c} = \cap_{k \leq m} A_{k,\delta}^c$. Conditional concentration of measure guarantees that the probability bounds in lemma 1 continue to hold; thus these sets capture ‘most’ realizations. Let $Q_p^m(\cdot)$, $p \in (0, 1)$, denote the quantile function retrieving the element in a vector $x \in \mathbb{R}^m$ that is greater than or equal to pm elements. Then on $A_\delta^{m,c}$, denoting $\lambda_m = (\lambda_1, \dots, \lambda_m)^T$ and $\|Y_m\|^2 = (\|Y_{\cdot 1}\|^2, \dots, \|Y_{\cdot m}\|^2)^T$,

$$(1 - \delta)\{Q_p^m(\lambda_m) + \sigma^2/m\} \leq Q_p^m(\|\mathbf{Y}_m\|^2/n) \leq (1 + \delta)\{Q_p^m(\lambda_m) + \sigma^2/m\}.$$

If p is fixed, by the decay assumption (6), we have $Q_p^m(\lambda_m) \asymp \{(1 - p)m\}^{-(2\alpha+1)}$, i.e. $m Q_p^m(\lambda_m) \propto m^{-2\alpha}$. Hence, on A_δ^c for some $0 < c \leq C$,

$$(1 - \delta)(\sigma^2 + cm^{-2\alpha}) \leq m Q_p^m(\|\mathbf{Y}_m\|^2/n) \leq (1 + \delta)(\sigma^2 + Cm^{-2\alpha}).$$

This motivates an estimator of σ^2 with small relative error on sets of high probability:

$$\hat{\sigma}_p^2 = m Q_p^m(\|\mathbf{Y}_m\|^2/n). \quad (19)$$

Further, we show that this holds for any p satisfying $\{(1 - p)m\}^{-(2\alpha+1)} = o(m^{-1})$. Thus we may let p vary to reveal an interesting phenomenon stated in the following theorem, with the proof deferred to the on-line supplementary material. To state the theorem more precisely, for $p \in (0, 1)$, we take $\hat{\sigma}_p^2 = m Q_p^m(\|\mathbf{Y}_m\|^2/n)$ and amend the Stein weights in expression (9),

$$\alpha_{mn,k}(\hat{\sigma}_p^2) = \left[1 - [1 + (q_\delta + 2)\sqrt{\{12 \log(m)/n\}}] \frac{n\hat{\sigma}_p^2/m}{\|Y_{\cdot k}\|^2} \right]_+, \quad (20)$$

where $q_\delta = (1 + 2\delta)/(1 - \delta) \gtrsim 1$ and $\delta = \sqrt{\{12 \log(m)/n\}}$. Corresponding estimates are formed as $\hat{\sigma}_{(p)}^2 = \hat{\sigma}_p^2$ if $p \leq 1/n$ and 0 otherwise.

Theorem 5.

In the case of L^2 -recovery, these are equivalent to the multiple GSMs (4) when projected onto the Karhunen–Loève (KL) basis (i.e. eigenfunctions) of the covariance function $C = \mathbf{E}(f \otimes f)$. Noting that the variances of the effects, λ_k , are non-decreasingly ordered eigenvalues in this setting, the decay condition $\lambda_k \propto k^{-(2\alpha+1)}$ in expression (6) is satisfied under fairly general assumptions. For instance, it is sufficient that C satisfies the Sacks–Ylvisacker conditions of order $r = \alpha - \frac{1}{2} \geq 0$ (Ritter *et al.*, 1995).

We see that, to apply the proposed recovery strategy to functional data, an obstacle is the unknown KL basis. Although this basis may be estimated from data, it is not our purpose to employ traditional functional principal component procedures, which are computationally expensive and introduce data-dependent uncertainty. Instead, we further extend the proposed Stein estimates and their theoretical guarantees to more general settings where the effects θ_{ik} may be correlated across k . This allows projection of the white noise models (21) onto other bases, such as wavelet or Fourier, provided that the correlation between projected coefficients satisfies some mild conditions.

Besides theoretical advantages, a major benefit of recovering functional data by GSMs is potentially significant computational savings. Typical presmoothing (Ramsay and Silverman, 2005) or post-smoothing (Yao *et al.*, 2005) of individual functions for estimation of covariance–eigenstructure operates with $O(nm^2 + m^3)$ complexity for common design, which scales poorly with data, and $O(n^3m^3)$ complexity for random design, which is intractable for large data sets. A recent proposal by Xiao *et al.* (2016) dealing with covariance estimation for functional data in common design settings using penalized splines operates at the order of $O(nm^{1+\rho})$, where $0 < \rho \leq 1$ depends on smoothness. In contrast, by our method we can take advantage of transforms, such as fast wavelet or Fourier transforms, to obtain recoveries in $O\{nm \log(m)\}$ time with spatial (or frequency) adaptation which capture striking features (Donoho and Johnstone, 1994), such as those illustrated in Fig. 1(b) in Section 4.1 later. A simple calculation indicates that our recovery strategy retains at most

$$d_* \lesssim [m\sqrt{\{n/\log(m)\}}]^{1/(2\alpha+1)}$$

non-zero weights with high probability. We may in turn run principal components analysis on these at $O(nd_*^2 + d_*^3)$ cost to attain estimates of the covariance–eigenstructure. The entire procedure may then potentially scale at $O\{nm \log(m)\}$. Further, our method may be employed in an on-line algorithm fashion: a new curve comes in; transform is performed; threshold weights are updated. This could potentially extend the FDA applications to realtime data collection and processing.

3.1. Review of Le Cam equivalence for non-parametric experiments

We begin with the notion of Le Cam equivalence that was used in Brown and Low (1996), Brown *et al.* (2002) and Reiß (2008), following an amalgam of notation from these sources. Denote two sequences of experiments by standard probability triples, indexed by an identical parameter space Θ_m , changing with m (or n), by

$$\begin{aligned}\mathbb{E}_m &= \{(\mathcal{X}_1^m, \mathcal{B}_1^m, P_{1,\theta}^m), \theta \in \Theta_m\}, \\ \mathbb{G}_m &= \{(\mathcal{X}_2^m, \mathcal{B}_2^m, P_{2,\theta}^m), \theta \in \Theta_m\}.\end{aligned}$$

Given randomized decision rules, δ^i , $i = 1, 2$, on a common action space \mathcal{A} and loss functions $L = L_m: \Theta_m \times \mathcal{A} \rightarrow [0, \infty)$, the corresponding risks, $R^i(\delta^i, L, \theta) = \mathbf{E}_{P_{i,\theta}^m}\{L(\delta^i, \theta)\}$, take the form

With the pseudonorm $\|L\| = \sup\{L(\theta, a) : \theta \in \Theta_m, a \in \mathcal{A}\}$, the experiments \mathbb{E}_m and \mathbb{G}_m are considered asymptotically equivalent in the Le Cam sense as $m \rightarrow \infty$, if

$$\Delta(\mathbb{E}_m, \mathbb{G}_m) := \max \left\{ \inf_{\delta^1} \sup_{\delta^2} \sup_{\theta \in \Theta_m, \|L\|=1} |R^1(\delta^1, L, \theta) - R^2(\delta^2, L, \theta)|, \right. \\ \left. \inf_{\delta^2} \sup_{\delta^1} \sup_{\theta \in \Theta_m, \|L\|=1} |R^1(\delta^1, L, \theta) - R^2(\delta^2, L, \theta)| \right\} \rightarrow 0. \quad (22)$$

To unify results on equivalence for fixed and random designs of non-parametric experiments, we need to introduce some background and notation on piecewise constant approximations. For a given positive integer k , let $I_{k,j} = [j/k, (j+1)/k)$ for $j=0, \dots, k-1$ and $I_{k,k-1} = [1-1/k, 1]$ so that the $I_{k,j}$ form a partition of $[0, 1]$. Let $\phi_{k,j} = k^{1/2} \mathbf{1}_{I_{k,j}}$, such that for a given k these functions form an orthonormal basis for the subspace S_k of $L^2[0, 1]$ consisting of functions that are constant on each of the $I_{k,j}$. The functions $H_{l,j} = 2^{-l/2}(\phi_{2^{l+1}, 2j} - \phi_{2^{l+1}, 2j+1})$, $l \geq 1$ and $k=0, \dots, 2^l - 1$, together with $H_{0,0} = \mathbf{1}_{[0,1]}$, form the orthonormal Haar wavelet basis of $L^2[0, 1]$ and $w_{l,j}(f) = \langle f, H_{l,j} \rangle$ the Haar wavelet coefficients for a function $f \in L^2[0, 1]$. We introduce a class of norms defined on the Haar wavelet coefficients, for a given $\alpha > \frac{1}{2}$,

$$\|f\|_{(\alpha)} = \left\{ \sum_{k=0}^{\infty} 2^{2k\alpha} \sum_{l=0}^{2^k-1} w_{k,l}^2(f) \right\}^{1/2},$$

which are closely related to a specific instance of Besov norms and provide a generalization of various types of smoothness, e.g. Hölder continuity or Sobolev smoothness. With these norms in place, we define the parameter spaces of interest. For some $B_n \rightarrow \infty$, we take

$$\Theta_m = \{f \in L^2[0, 1] : \|f\|_{(\alpha)} < B_m\}.$$

Now let \mathbb{F}_m and \mathbb{R}_m denote the non-parametric experiments in model (2) for fixed and random designs respectively, and let \mathbb{W}_m denote the white noise model (3), as f ranges over Θ_m . The following lemma provides a generalization of existing results that may be applied to functional data models; see the on-line supplementary material for its proof.

Lemma 2. For fixed and random designs of the non-parametric experiments (2), we have a unified bound on the Le Cam distance

$$\max\{\Delta(\mathbb{F}_m, \mathbb{W}_m), \Delta(\mathbb{R}_m, \mathbb{W}_m)\} \lesssim B_m^2 m^{-(2\alpha-1)/(2\alpha+1)}.$$

Consequently, if $B_m = o(m^{(2\alpha-1)/(4\alpha+2)})$, we have the asymptotic equivalence in Le Cam sense between the non-parametric model (2) under both designs and the white noise model (3).

3.2. Functional data and white noise representations

Given a single function f as a realization of a sufficiently smooth stochastic process, we may form the non-parametric regression experiment $y_i = f(x_i) + z_i$ and corresponding white noise model $Y(dt) = f(t)dt + m^{-1/2}W(dt)$, $i = 1, \dots, m$. It is not obvious that we may approximate the random variables $\mathbf{E}_f\{L(f, \cdot)\}$ from one model by those from the other as $m \rightarrow \infty$. Modulo proper assumptions on the smoothness of f , this is indeed possible and can be shown by using Le Cam equivalence theory for fixed functions, e.g. lemma 2 from above. Intuitively, this works because, for reasonable stochastic processes, the smoothness of f measured in $\|\cdot\|_{(\alpha)}$ has null probability of growing sufficiently fast as $m \rightarrow \infty$ to dominate the convergence rate of Le Cam equivalence of the experiments over Θ_m . By extension, it is not obvious that, given n non-

parametric regression models sampled at m points generated from the functional data model (5), the risks $\mathbf{E}_{f_i}\{L(f_i, \cdot)\}$, $i = 1, \dots, n$, from the non-parametric regression models are approaching those from the corresponding white noise models (21).

Recall that n and m are asymptotically linked through the constraint $m^{\gamma_1} \lesssim n \lesssim m^{\gamma_2}$. The main appeal of lemma 2 is that proving bounds on wavelet coefficients $|w_{i,j}(f)|$ under various smoothness constraints that are commonly used in practice is a relatively simple task, whereas in FDA smoothness constraints are typically imposed through moment conditions on a norm $\|f\|^*$ which often dominates $\|f\|_{(\alpha)}$ for some $\alpha > \frac{1}{2}$. If the growth of the norms $\max_{i \leq n} \|f_i\|^*$ can be controlled almost surely by a B_m satisfying the conditions of lemma 2, we may construct a Θ_m over which we have Le Cam equivalence between the experiments of the previous section while ensuring that eventually $f_1, \dots, f_n \in \Theta_m$. This means that for any estimator δ^1 in the non-parametric regression experiment there is an estimator δ^2 in the white noise model, and vice versa, so that eventually

$$\begin{aligned} \max_{1 \leq j \leq n} \sup_{\|L\| \leq 1} |R^1(\delta^1, L, f_j) - R^2(\delta^2, L, f_j)| &\leq \sup_{f \in \Theta_m} \sup_{\|L\| \leq 1} |R^1(\delta^1, L, f) - R^2(\delta^2, L, f)| \\ &\lesssim B_m^2 m^{-(2\alpha-1)/(2\alpha+1)} = o(1). \end{aligned}$$

As this allows for randomized estimators, we are guaranteed that we can model functional data (5), under risks $\mathbf{E}_{f_i}\{L(f_i, \cdot)\}$, by the corresponding risks under white noise models (21), and vice versa. This follows on noting that $\mathbf{E}_{f_i}(\cdot) = \mathbf{E}(\cdot | f_i)$ is the expectation that averages over all data in $j \neq i$ experiments and the noise in the i th experiment, and thus any estimator which pools over $j = 1, \dots, n$ may be viewed as a randomized estimator with respect to \mathbf{E}_{f_i} . We first provide a useful lemma and some concrete examples and then summarize in a general theorem.

Lemma 3. Suppose that $f \in L^2[0, 1]$ has a generalized derivative $f' \in L^2[0, 1]$. Then $w_{0,0}^2(f) \leq \|f\|_2^2$ and, for $k \geq 1$, $l = 0, \dots, 2^k - 1$, the Haar wavelet coefficients obey the decay

$$w_{k,l}^2(f) \leq 2^{-2k} \int_{I_{k,l}} |f'(s)|^2 ds.$$

Consequently, $\|f\|_{(\alpha)} < \infty$ for any $\alpha \in (\frac{1}{2}, 1)$ and may be bounded by a factor of $\|f\|_2 + \|f'\|_2$ which may, in turn, be bounded by a factor of $|f(0)| + \|f'\|_2$.

On the basis of lemma 3 and the discussion above, if the growth of the norms $\max_{i \leq n} (\|f_i\| + \|f'_i\|_2)$ can be controlled almost surely by $m^{-(2\alpha-1)/(2\alpha+1)}$, we may construct a Θ_m over which we have Le Cam equivalence between the experiments while ensuring eventually $f_1, \dots, f_n \in \Theta_m$.

3.2.1. Example 1

A general method for forming processes is to smooth white noise by integrating against a kernel. Regularity assumptions on the underlying kernel result in regularity of the sample paths. As a concrete example, suppose that all second-order partial derivatives of $R: [0, 1]^2 \rightarrow \mathbb{R}$ exist and are of bounded variation with either argument taken as fixed. Define the process f on $[0, 1]$ by $f(s) = \int_0^1 R(s, t) B(dt)$, where B is Brownian motion. First note that $f(0)$ is Gaussian with mean 0 and, by Ito isometry, variance $\int_0^1 R^2(0, t) dt$, which gives $\max_{i \leq n} |f_i(0)| \lesssim \log(m)^{1/2}$ almost surely under the assumptions on n and m . Further, the assumptions on R allow us to integrate by parts $f'(s) = B(1) \partial_s R(s, 1) - \int_0^1 B(t) \partial_s R(s, dt)$. Denoting the variation of a function g by $V(g, [0, 1])$ gives

$$\|f'\|_\infty \leq \sup_{0 \leq s \leq 1} [|\partial_s R(s, 1)| + V\{\partial_s R(s, \cdot), [0, 1]\}] \sup_{0 \leq t \leq 1} B(t).$$

If the first supremum term is bounded, the reflection principle puts sub-Gaussian tails on $\|f'\|_\infty$. Hence, for a sample $f_1, \dots, f_n \sim^{\text{IID}} f$, we have $\max_{i \leq n} \|f'_i\|_\infty \lesssim \log(m)^{1/2}$, almost surely. Since $m^{-(2\alpha-1)/(2\alpha+1)} \log(m) = o(1)$ for any choice of $\alpha \in (\frac{1}{2}, 1)$, lemma 2 gives Le Cam equivalence over $\Theta_m = \Theta_m(\alpha)$ with $B_m \lesssim \log(m)^{1/2}$. Lemma 3 implies that $\|f\|_{(\alpha)} \lesssim |f(0)| + \|f'\|_2$ which is bounded by $|f(0)| + \|f'\|_\infty$. This guarantees that, in view of $\max_{i \leq n} (|f_i(0)| + \|f'_i\|_\infty) \lesssim \log(m)^{1/2}$ almost surely; we eventually have $f_1, \dots, f_n \in \Theta_m$. Thus we may model the risks of recovering the f_i from functional data by white noise models. Sufficiently regular convolutions fall under this model, which generalizes to processes formed by taking linear combinations of this form.

3.2.2. Example 2

Slightly more general assumptions in the FDA literature include, for all $C > 0$,

$$\max_{j=0,1,2} \mathbf{E} \|f^{(j)}\|_\infty^C < \infty,$$

as in Hall *et al.* (2006). A weakening of this requirement which might be seen as a strengthening of the condition in Cai and Yuan (2011) requires, for all $C > 0$,

$$\max_{j=0,1,2} \mathbf{E} \|f^{(j)}\|_2^C < \infty.$$

Under these conditions, for any choice of $\alpha \in (\frac{1}{2}, 1)$ and a sample $f_1, \dots, f_n \sim^{\text{IID}} f$, we have

$$\max_{i \leq n} (\|f_i\|_2 + \|f'_i\|_2) = o_{a.s.}(m^{-(2\alpha-1)/(2\alpha+1)}).$$

Thus, as in the previous example, we may model the risks of recovering the f_i from functional data by white noise models.

These examples indicate a general approach to establishing validity of white noise equivalence for functional data, as stated in the following theorem with proof in the on-line supplementary material, which includes the commonly adopted settings in the FDA literature as special cases. Recall the general setting $m^{\gamma_1} \lesssim n \lesssim m^{\gamma_2}$ for any $\gamma_2 \geq \gamma_1 > 0$, and the decay parameter $\alpha > 0$ in expression (6).

Theorem 6. Suppose that for a norm $\|\cdot\|^*$ which dominates $\|\cdot\|_{(\alpha)}$ for some $\alpha \in (\frac{1}{2}, 1)$, as in the examples above, the process f satisfies

$$\mathbf{P}(\|f\|^* > x) \lesssim (1+x)^{-\beta},$$

for some $\beta > 2(\alpha+1) \max(1, \gamma_2)/(2\alpha-1)$. Then we can model the recovery of functional data in both fixed and random designs, by white noise models (23).

3.3. Recovery of functional data in general basis and extension to general decay

A remaining issue of applying the recovery strategy to functional data is that the multiple GSMs (4) assume independence between θ_{ik} across k , which corresponds to projecting white noise models (21) onto the unknown KL basis of $C = \mathbf{E}(f \otimes f)$. We elaborate that, for projections onto other bases with the coefficients displaying to some extent decaying correlations, the recovery results continue to hold modulo constants and yield estimators that are adaptive to the average case oracle strategies.

We are now dealing with the case that the coefficients θ_{ik} are projections of f_i onto a given basis ψ_k , $\theta_{ik} = \langle f_i, \phi_k \rangle$. Given the independence across curves, the oracle inequality of theorem

1 continues to hold and the main difficulty lies in generalizing the results of theorem 2 to deal with dependence between the projected coefficients of the underlying process. With $\lambda_k = \text{var}(\theta_{ik})$, set

$$\left. \begin{aligned} \Delta_m &= \text{diag}(\lambda_1, \dots, \lambda_m), \\ \Sigma_m &= (\text{cov}(\theta_{ij}, \theta_{ik}))_{j,k \leq m}, \\ \Gamma_m &= \Delta_m^{-1/2} \Sigma_m \Delta_m^{-1/2}. \end{aligned} \right\} \quad (23)$$

The matrix Γ_m provides termwise correlations between projected coefficients in the chosen basis, $\{\psi_k\}_{k=1}^\infty$ and reduces to the identity for KL basis.

The following conditions are sufficient to guarantee that our procedure recovers θ_i at the optimal rate.

Condition 1. The ordered variances $\lambda_k = \text{var}(\theta_{ik})$ decay as $\lambda_{(k)} \propto k^{-(2\alpha+1)}$.

Condition 2. The correlations between θ_{ik} decay sufficiently fast that

$$\max_{i \leq m} \sum_{j=1}^m |\Gamma_{m,ij}| \leq B_m. \quad (24)$$

with $B_m^2 = O\{m^{1/(2\alpha+1)} / \log(m)^p\}$ for some $p \geq 2$.

Remark 3. Regarding condition 1, it is known that covariance functions satisfying the Sacks–Ylvisacker conditions of order $r = \alpha - \frac{1}{2}$ generate reproducing kernel Hilbert spaces lying within a polynomial translation of the Sobolev space $H^{r+1}([0, 1])$. There are many comparable smoothness classes which share similar decay when expressed in efficient bases. Thus it is reasonable to expect that in such bases $\lambda_{(k)}$ decay at the KL rate, which does not know the ordering *a priori*.

$$\sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} \frac{\text{cov}(\theta_{jk}, \theta_{pq})}{\sqrt{\{\text{var}(\theta_{jk})\text{var}(\theta_{pq})\}}} \leq B.$$

3.3.2. Example 4: Sobolev reproducing kernel and smooth wavelet basis

Let K_r , $r \in \mathbb{N}$, be the reproducing kernel of order r , given by $K_r(x, y) = A(x, y) + B(x, y)$,

$$A(x, y) = \sum_{p=0}^r \frac{x^p y^p}{(p!)^2},$$

$$B(x, y) = \int_0^{\min(x, y)} \frac{(x-u)^r (y-u)^r}{(r!)^2} du,$$

which is a polynomial of order $2r+1$ in x and y . This is the canonical example of covariance structure for a process satisfying Sacks–Ylvisacker conditions of order r . Let f be a mean 0 Gaussian process with the covariance kernel K_r , and $\{\psi_{jk}\}_{j,k}$ be a compactly supported wavelet basis orthogonal to polynomials of degree $2r+1$. The next proposition indicates that the recovery holds for such processes with $B_m \lesssim \log(m)$, noting the scales $p \lesssim \log(m)$ in wavelet bases.

Proposition 2. In the setting outlined above, the covariance structure of the wavelet coefficients θ_{jk} satisfies

$$\frac{\text{cov}(\theta_{jk}, \theta_{j'k'})}{2^{-(r+1)(k+k')}} = \begin{cases} 0, & \text{supp}(\psi_{jk}) \cap \text{supp}(\psi_{j'k'}) = \emptyset, \\ O(2^{-(r+1/2)|k-k'|}), & \text{otherwise.} \end{cases}$$

Consequently, for fixed p and q and some $B > 0$,

$$\sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} \frac{\text{cov}(\theta_{jk}, \theta_{pq})}{\sqrt{\{\text{var}(\theta_{jk})\text{var}(\theta_{pq})\}}} \leq B \max(1, p).$$

Remark 4. We expect that the above examples hold in greater generality. For instance, in the stationary example, given the local nature of ψ_{jk} for general wavelet bases of $L^2[0, 1]$, it is reasonable to expect that similar decay conditions are satisfied if f is taken as a ‘snapshot’ over $[0, 1]$ of a process over \mathbb{R} corresponding to K of a locally stationary process as in Mallat *et al.* (1998). Similarly, the derivation for Sobolev-type kernels extends to $A(x, y)$ with reasonable coefficients, and $B(x, y)$ may be expanded to include integrals against more general functions of u .

3.3.3. Example 5: Calderon–Zygmund and pseudodifferential-type integral operators and sufficiently regular wavelet basis

More generally, in sufficiently regular wavelet bases $\{\psi_{jk}\}_{j,k}$, integral operators C such as Calderon–Zygmund and pseudodifferential type, which correspond to broad classes of covariance structures, are known to satisfy decay conditions of the form

$$|\langle \psi_{jk}, C\psi_{j'k'} \rangle| \lesssim \frac{2^{-(r+1)(j+j')} \times 2^{-\kappa|j-j'|}}{[1 + d\{(j, k), (j', k')\}]^\gamma},$$

where $d\{(j, k), (j', k')\} = 2^{\min(j, j')} |2^{-j}k - 2^{-j'}k'|$ provides a measure of plei 0 21 Tf between 666 -1.2 8074

covariance structure of the wavelet coefficients θ_{jk} , and thus $B_m \lesssim \log(m)$ with $p \lesssim \log(m)$ in wavelet bases.

Proposition 3. In the setting outlined above, the covariance structure of the wavelet coefficients θ_{jk} satisfies, for fixed p and q ,

$$\sum_{j=0}^{\infty} \sum_{k=0}^{2^j-1} \frac{\text{cov}(\theta_{jk}, \theta_{pq})}{\sqrt{\{\text{var}(\theta_{jk})\text{var}(\theta_{pq})\}}} \lesssim p.$$

Further, if $\gamma > 1$ this bound is constant and independent of m .

We conclude this section by pointing out that the results of this paper can be extended to more general decay settings. Denote by \mathcal{R} the average oracle risk, $\mathcal{R} = \mathcal{R}(m) = \sum_{k=1}^{\infty} (\lambda_k/m)(\lambda_k + 1/m)$. The following conditions are needed for the method proposed to continue to hold.

Condition 3. The signal in the components larger than noise, $\lambda_k > 1/m$, dwarfs the operator norm of the correlations, i.e. $(m\mathcal{R})/\|\Gamma\|^2 \gtrsim \log(m)^2$.

Condition 4. The bulk of signal components larger than noise, $\lambda_k > 1/m$, remain in the first m components, i.e. $\sum_{k>m} \lambda_k = o\{\mathcal{R}/\log(m)\}$.

Condition 5. The risk is slowly varying in m so that $\mathcal{R}(m/\delta) \lesssim \delta^\gamma \mathcal{R}(m)$ for some $\gamma \in (0, 1)$.

It is easy to verify that a more general decay $k^{-(2\kappa+1)} \lesssim \lambda_{(k)} \lesssim k^{-(2\alpha+1)}$ with λ_k slowly varying for $k \leq m$ and $k^{-(2\kappa+1)} \lesssim \lambda_k \lesssim k^{-(2\alpha+1)}$ for $k > m$, where $0 < \alpha < \kappa$, satisfies these conditions.

Theorem 8. Consider multiple GSMs (4) with conditions 3–5 holding, and suppose that $n, m \rightarrow \infty$ with $m^{\gamma_1} \lesssim n \lesssim m^{\gamma_2}$ for any $\gamma_2 \geq \gamma_1 > 0$. Then the method proposed continues to adapt to the average case oracle, i.e. $\max_{i \leq n} \mathbf{E} \theta_i \|\theta_i - \hat{\theta}_i\|_{L_2}^2 / \mathcal{R} = 1 + o(1)$ almost surely.

4. Simulated and real data examples

In this section, we first report simulation experiments which highlight advantages of information pooling in multiple GSMs. The performance of our recovery procedure is compared against the linear oracle as well as individual blocking and soft thresholding estimators. Robustness to deviation from distributional assumptions and model complexity associated with estimation of σ^2 are also examined, with results supporting our theoretical findings. We then apply the proposed method to the phoneme data set that was studied in Hastie *et al.* (1995). Classification performance and computational times of our method are compared against those attained by common FDA methods based on pre- or post-smoothing individual functions.

4.1. Simulation studies

The simulated data are generated from the multiple GSMs with the first m effects,

$$Y_{ik} = \theta_{ik} + m^{-1/2} z_{ik}, \quad k = 1, \dots, m, \quad i = 1, \dots, n, \quad (25)$$

where $z_{ik} \sim \text{iID } N(0, 1)$, $\theta_{ik} \sim N(0, \lambda_j) \perp z_{ik}$ and two scenarios are considered. The first scenario follows the model where variances λ_k are decreasing in k with Sobolev-type decay $\lambda_k = \lambda_{(k)} = 2\alpha k^{-(2\alpha+1)}$. In the second scenario, we permute $\{\lambda_k\}_{k \leq m}$ uniformly at random and then generate data from the model according to the permuted sequence. In each scenario, 1000 Monte Carlo runs are performed for all combinations of sample sizes $n = 10, 100, 1000$, sampling rates $m = 50, 500, 5000$ and decay speeds $\alpha = \frac{2}{3}$ and $\alpha = 1$. The benchmark is the linear oracle $\hat{\theta}_{ik}^{o,a} =$

$\lambda_k Y_{ik}/(\lambda_k + \sigma^2/m)$. For the method proposed, we calculate the Stein weights by using both true and estimated variances, i.e. $\alpha_{mn,k}$ in expression (9) with the true value $\sigma^2 = 1$, $\alpha_{mn,k}(\hat{\sigma}_{\min}^2)$ in expression (20) with q_δ in expression (5) and $\hat{\sigma}_{\min}^2 = (m\|\mathbf{Y}_m\|^2/n)_{(m)}$. To highlight advantages of information pooling, we also compare with the ‘individual’ blocking and soft thresholding estimators, denoted by $\hat{\theta}_i^B$ and $\hat{\theta}_i^{\text{ST}}$ respectively, using $\sigma^2 = 1$. Note that both methods use only the data $\{Y_{ik}\}_{k \leq m}$ from the i th experiment to estimate the effects θ_i . Specifically, we use the weakly geometric blocking scheme for $\hat{\theta}_i^B$ and the threshold level $\sqrt{\{2 \log(m)\}}$ for $\hat{\theta}_i^{\text{ST}}$. See Tsybakov (2009) and Donoho and Johnstone (1994) for explicit formulae.

Shown in Table 1 are the average and maximal l^2 -errors over n recoveries, $\{\|\theta_i - \hat{\theta}_i\|_{l_2}^2\}_{i \leq n}$, for both decreasing and permuted $\{\lambda_k\}_{k \leq m}$ by using different methods with the decay parameter $\alpha = \frac{2}{3}$. The results provide empirical evidence for the assertions in theorem 2 and demonstrate the advantage of information pooling across experiments by our method, using both true and estimated variance, even when the sample size is moderate at $n = 100$. It is expected that the blocking method performs well for the case of decreasing $\{\lambda_k\}_{k \leq m}$ with a large sampling rate,

Table 1. Average and maximal l^2 -errors over n recoveries, $\{\|\theta_i - \hat{\theta}_i\|_{l_2}^2\}_{i \leq n}$, for both decreasing and permuted sequences of $\{\lambda_k\}_{k \leq m}$ using various methods, when the decay parameter $\alpha = \frac{2}{3}$ and the sampling rate m varies

| m | Method | Results ($\times 10^2$) for $n = 10$ | | Results ($\times 10^2$) for $n = 100$ | | Results ($\times 10^2$) for $n = 1000$ | |
|---|---|--|---------|---|---------|--|---------|
| | | Average | Maximum | Average | Maximum | Average | Maximum |
| <i>Decreasing sequence $\ell^{\lambda_k} \lambda_{k \leq m}$</i> | | | | | | | |
| 50 | Oracle $\hat{\theta}_i^{\text{o,a}}$ | 15.4 | 25.6 | 15.2 | 35.3 | 15.2 | 44.8 |
| | $\hat{\theta}_i^{\text{RS}}(\sigma^2)$ | 32.4 | 60.7 | 21.3 | 50.3 | 16.9 | 48.2 |
| | $\hat{\theta}_i^{\text{RS}}(\hat{\sigma}_{\min}^2)$ | 21.5 | 36.9 | 20.9 | 49.2 | 17.4 | 49.3 |
| | Block $\hat{\theta}_i^{\text{B}}$ | 21.5 | 37.2 | 21.4 | 51.1 | 21.4 | 64.7 |
| | Soft $\hat{\theta}_i^{\text{ST}}$ | 46.3 | 77.2 | 46.1 | 101 | 46.1 | 123 |
| 5000 | Oracle $\hat{\theta}_i^{\text{o,a}}$ | 1.19 | 1.46 | 1.19 | 1.66 | 1.19 | 1.83 |
| | $\hat{\theta}_i^{\text{RS}}(\sigma^2)$ | 2.88 | 3.78 | 1.84 | 2.64 | 1.39 | 2.11 |
| | $\hat{\theta}_i^{\text{RS}}(\hat{\sigma}_{\min}^2)$ | 9.88 | 10.5 | 1.60 | 2.25 | 1.39 | 2.11 |
| | Block $\hat{\theta}_i^{\text{B}}$ | 1.58 | 1.99 | 1.58 | 2.28 | 1.58 | 2.54 |
| | Soft $\hat{\theta}_i^{\text{ST}}$ | 5.97 | 7.23 | 5.97 | 8.08 | 5.97 | 8.76 |
| <i>Permuted sequence $\ell^{\lambda_k} \lambda_{k \leq m}$</i> | | | | | | | |
| 50 | Oracle $\hat{\theta}_i^{\text{o,a}}$ | 15.3 | 26.0 | 15.2 | 35.5 | 15.2 | 44.7 |
| | $\hat{\theta}_i^{\text{RS}}(\sigma^2)$ | 32.3 | 61.0 | 21.3 | 50.3 | 16.9 | 47.9 |
| | $\hat{\theta}_i^{\text{RS}}(\hat{\sigma}_{\min}^2)$ | 21.4 | 36.8 | 20.9 | 49.0 | 17.4 | 49.1 |
| | Block $\hat{\theta}_i^{\text{B}}$ | 73.0 | 182 | 70.0 | 320 | 71.1 | 475 |
| | Soft $\hat{\theta}_i^{\text{ST}}$ | 46.0 | 76.7 | 46.2 | 101 | 46.1 | 122 |
| 5000 | Oracle $\hat{\theta}_i^{\text{o,a}}$ | 1.19 | 1.46 | 1.19 | 1.66 | 1.19 | 1.83 |
| | $\hat{\theta}_i^{\text{RS}}(\sigma^2)$ | 2.88 | 3.78 | 1.84 | 2.65 | 1.39 | 2.11 |
| | $\hat{\theta}_i^{\text{RS}}(\hat{\sigma}_{\min}^2)$ | 9.57 | 10.2 | 1.60 | 2.26 | 1.39 | 2.12 |
| | Block $\hat{\theta}_i^{\text{B}}$ | 53.7 | 146 | 53.7 | 270 | 51.5 | 376 |
| | Soft $\hat{\theta}_i^{\text{ST}}$ | 5.97 | 7.25 | 5.97 | 8.09 | 5.97 | 8.77 |

for instance $m = 5000$, but degrades substantially when λ_k are randomly permuted. Although soft thresholding is adaptive to permutation, it incurs much larger errors. Although variants of procedures tuned by Stein's unbiased risk estimation may fare better against ours, we consider it fair to compare our tuning-free method using a universal threshold with those requiring similar computation. The results of $\alpha = 1$ illustrate a similar performance pattern (which is not reported) with overall smaller errors, as faster decay corresponds to smoother functions that are easier to be recovered. To appreciate the adaptivity to permutation, we depict a realization θ_i and its random permutation in Figs 1(a) and 1(b), expanded in a smooth wavelet basis, specifically, the symlets of order 6, that is nearly symmetric with a minimum support size for that order corresponding to the number of vanishing moments. It is evident that the function corresponding to permuted effects exhibits striking local features and thus presents a more challenging pattern for recovery from a smoothness regularity perspective. We also inspect the robustness of the proposed method in the case of recovering new observations-generated distributions that violate the Gaussian assumption. The results, which are reported in Table S1 of the on-line supplementary material, provide an empirical support to theorem 4.

It is of also interest to examine the influence of quantiles on the estimation of σ^2 which manifests in a trade-off between quality of recovery and model complexity. We use data of size $n = m = 100$ for enhanced visualization with $\lambda_k = 2\alpha k^{-(2\alpha+1)}$ and calculate recoveries of $\{\theta_i\}_{i \leq n}$ by Stein estimation (20) using $\hat{\sigma}_p^2$ (19) over a range of percentages. From Fig. 1(c) showing the pattern of maximal recovery error as a function of p , as dictated by theorem 5, we observe an 'elbow'-type transition from consistency to a sudden risk hike, when p exceeds a certain threshold p^* approaching 1. Together with Fig. 1(d) showing the corresponding model complexity measured by the number of retained variables, we see that exercising caution in choosing a larger p may be worthwhile for balancing model complexity and quality of recovery.

4.2. Application to phoneme data

We apply our recovery method to the phoneme data set that was studied in Hastie *et al.* (1995). The data consist of $n = 4509$ equally spaced log-periodogram sequences of length $m = 256$ derived from continuous speech of male subjects. Each sequence of log-periodograms belongs to one of the five categories: 'sh', 'dcl', 'iy', 'aa' and 'ao'. To assess the classification performance, we randomly split the data into a training sample of 1000 trajectories *versus* a testing sample of 3509 for each of 100 Monte Carlo iterations. In each run, we perform three procedures on the training sample: penalized spline smoothing of individual functions (i.e. pre-smoothing; Ramsay and Silverman (2005)) followed by eigendecomposition of covariance, denoted by RAMS; the principal analysis through conditional expectation (PACE) method (Yao *et al.*, 2005) based on kernel smoothing to raw covariances formed from noisy data (i.e. post-smoothing); the proposed Stein estimation in a smooth wavelet basis, denoted by STEIN. For recoveries by this method, a periodized Battle-Lemarie wavelet system (spline based) with six vanishing moments was used. Then a simple linear discriminant classifier is fitted in the reduced model spaces, the functional principal component scores resulting from RAMS and PACE, and the coefficients retained from our method. For a comprehensive comparison over various model dimensions, we train the classification rules for the RAMS and PACE methods by retaining functional principal component that explain 90%, 95% and 99% of total variance, whereas different percentages for $\hat{\sigma}^2(p)$ are used in our method, specifically $p = 0.60, 0.70, 0.75, 0.80, 0.85, 0.90$. Results in Table 2 show that, although classification by each method appears indistinguishable in its optimal case and is also comparable with the benchmark in Hastie *et al.* (1995), our recovery method is seen to be much more stable over different complexities.

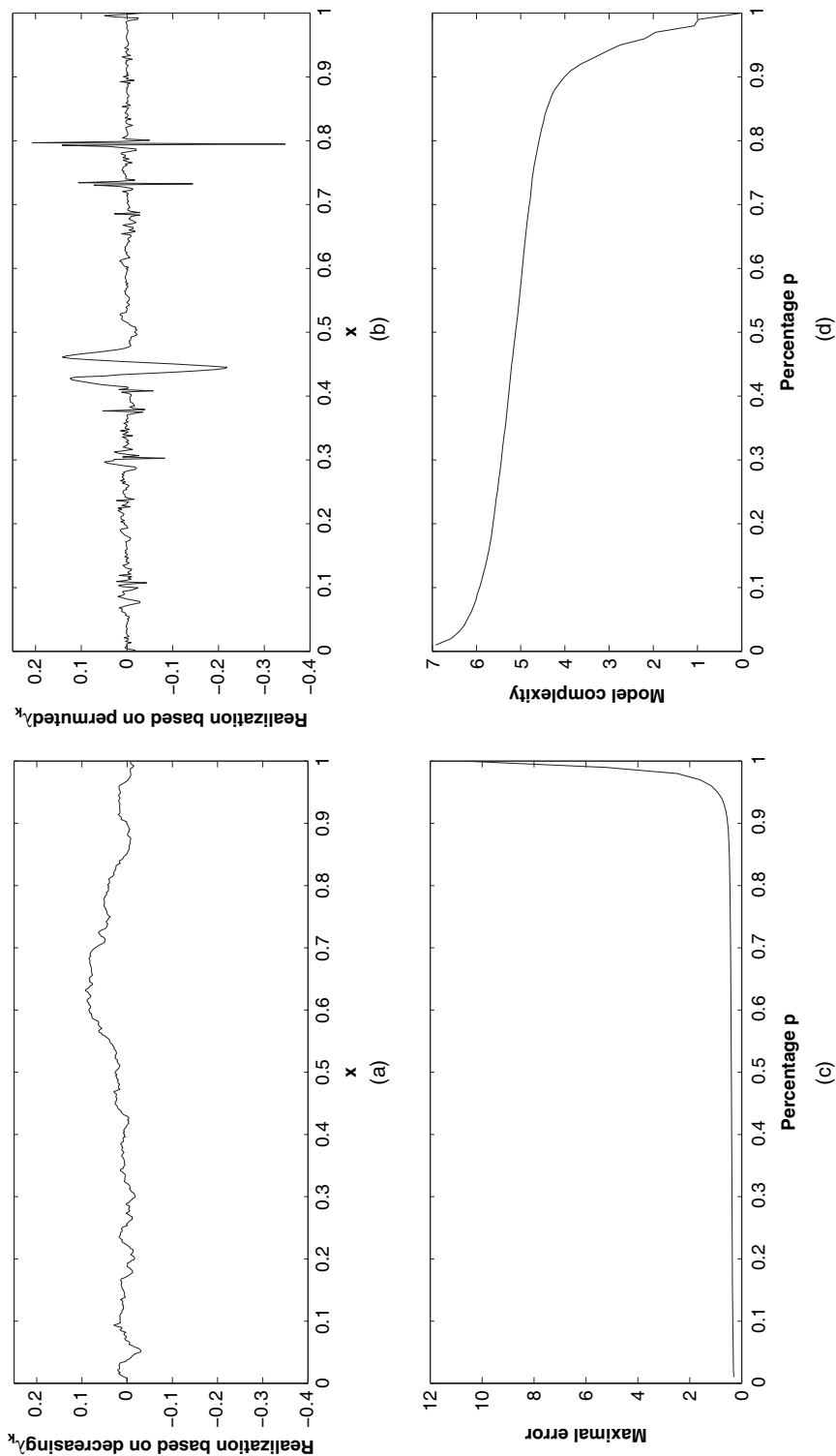


Fig. 1. A randomly chosen realization generated from (a) the decreasing and (b) the permuted sequences of $\{\lambda_k\}_{k \leq m}$ with $m = 500$, expanded in a smooth wavelet, and (c) the maximum error ($\times 10^2$) and (d) model complexity measured by the number of retained variables as functions of p used in σ_p^2 (19) respectively, when $n = m = 100$

Table 2. Classification error CE based on 100 random partitions of phoneme data into training ($n = 1000$) and testing ($N = 3509$) samples and model complexity determined by the percentage p in $\hat{\sigma}^2(p)$ for the method proposed (STEIN), and by the total variance explained, TVE, for the RAMS and PACE methods†

| STEIN | | | | | | |
|---|-------------|-------------|-------------|-------------|-------------|-------------|
| <i>Comparison of performance</i> | | | | | | |
| $\hat{\sigma}^2(p)$ | $p = 0.60$ | $p = 0.70$ | $p = 0.75$ | $p = 0.80$ | $p = 0.85$ | $p = 0.90$ |
| CE (%) | 7.66 (0.32) | 7.68 (0.33) | 7.85 (0.38) | 7.82 (0.35) | 7.48 (0.30) | 7.65 (0.30) |
| RAMS | | | PACE | | | |
| TVE | 90% | 95% | 99% | 90% | 95% | 99% |
| CE (%) | 10.9 (0.36) | 8.15 (0.46) | 7.72 (0.31) | 12.2 (0.60) | 9.25 (0.33) | 7.68 (0.33) |
| <i>Comparison of computation time (min)</i> | | | | | | |
| | $m = 512$ | $m = 1024$ | $m = 2048$ | $m = 4096$ | $m = 8192$ | $m = 16384$ |
| STEIN | 0.068 | 0.078 | 0.113 | 0.169 | 0.328 | 0.860 |
| RAMS | 0.108 | 0.240 | 0.664 | 3.76 | 26.5 | 221 |
| PACE | 6.95 | 30.2 | 98.9 | 426 | — | — |

†The average computation time is for a full sample ($n = 4509$) of extrapolated data by adding noise to recovered curves at increased sampling rates m .

To illustrate computational savings we use synthetic data, with recovered curves and estimated variance $\hat{\sigma}^2$ used to extrapolate the original data to larger sampling rates m . To be specific, we add noise following $N\{0, \hat{\sigma}^2(p)\}$ with $p = 0.9$ to the curves recovered by our method to generate larger synthetic data sets with $m = 512, 1024, 2048, 4096, 8192, 16384$. We use the public MATLAB packages at <http://www.psych.mcgill.ca/misc/fda> and <http://www.stat.ucdavis.edu/PACE> for the RAMS and PACE methods with default selections for smoothing parameters, on a Macintosh Minicomputer with a 2.3 GHz Intel Core i7 chip and 8 Gbytes of DDR3 random-access memory. The average computation times for one full sample of $n = 4509$ reported in Table 2 indicates significant time savings for large m regimes by the method proposed, which approximately agree with the computation complexity: $O(nm^2 + m^3)$ for RAMS, $O(nm^2 + m^6)$ for PACE and $O\{nm + m \log(m)\}$ for our method. Note that the PACE method is designed for sparse functional data with random design and thus encounters computational challenges in dense designs when data are not binned before smoothing.

5. Potential application to other statistical problems

The statistical principles and mathematical techniques that are explored in this paper may be lent to broad classes of problems involving information pooling across similar experiments. An example is the change point problem that has been traditionally treated individually (Fryzlewicz, 2014, 2016). More recently, the change point problem has been considered in the context of panel data where common structure lends strength to multiple-change-point detection (Cho, 2016). We briefly outline a treatment of multiple change points for panel data through the lens of multiple GSMs, which may deserve a further study.

Assume that the data consist of $Y_{ij} = \theta_{ij} + z_{ij}$, $i = 1, \dots, n$ and $j = 1, \dots, m + 1$, with θ_{ij} varying independently across i (individuals) and being piecewise constant across j (time) with T (unknown) change points at $k_l \in \{2, \dots, m + 1\}$, $l = 1, \dots, T$. At the unknown change points, assume that the $\theta_{ij} \sim N(0, \lambda)$ are generated independently of each other and are also independent

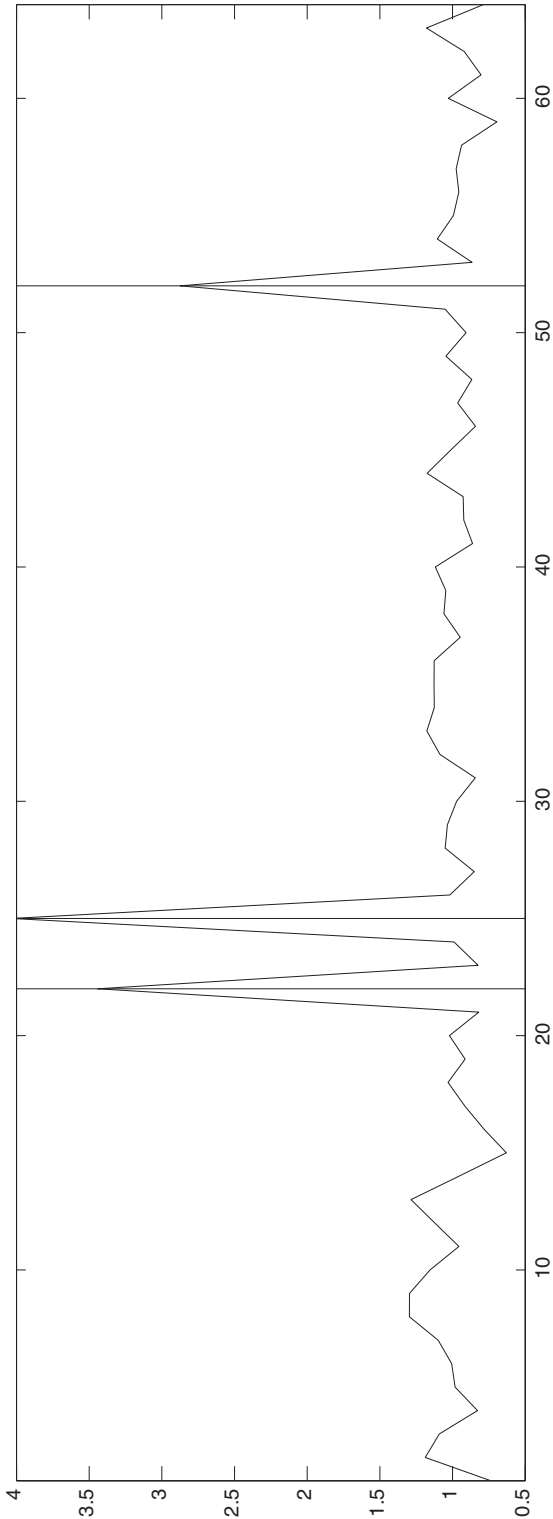


Fig. 2. Ratios $\|Y_{i,\cdot}^*\|^2 / \text{med}(\|Y_{i,\cdot}^*\|^2)$ for one Monte Carlo sample with $n = 100$, $m = 64$, $\lambda = 3$ and change points at $j = 22, 25, 52$; |, successful detection of the change points

of the z_{ij} which are independent and identically distributed $N(0, 1)$. We difference the data to form GSMs, denoting $Y_{ij}^* = Y_{i,j+1} - Y_{ij}$ and similarly θ_{ij}^* and z_{ij}^* ,

$$Y_{ij}^* = \theta_{ij}^* + z_{ij}^*, \quad i = 1, \dots, n, \quad j = 1, \dots, m.$$

Note that $\theta_{ij}^* = 0$ except at the unknown change points in which case $\theta_{ij}^* \sim N(0, 2\lambda)$ and $z_{ij}^* \stackrel{\text{iid}}{\sim} N(0, 2)$. Thus we have $\|Y_{\cdot j}^*\|^2 \approx 2n(1 + \lambda)$ for $j \in \{k_1, \dots, k_T\}$ and $2n$ otherwise. Applying the proposed Stein procedure to estimate θ_{ij}^* , we find that $\hat{\theta}_{ij}^*$ are non-zero, with high probability, at the locations satisfying

$$\|Y_{\cdot j}^*\|^2 / (2n) > 1 + 2\delta,$$

whenever $\lambda > (1 + 2\delta)(1 + \delta)/(1 - \delta) - 1 = o(1)$. Shown in Fig. 2 is an illustration of $\|Y_{\cdot j}^*\|^2 / (n\hat{\sigma}^2)$ with $n = 100$, $m = 64$ and $\lambda = 3$ in a Monte Carlo sample, where we take the median $\hat{\sigma}^2 = n^{-1} \text{med}(\|Y_{\cdot j}^*\|^2)$. Moreover, we have successfully detected the three change points in nearly all the 100 Monte Carlo samples.

6. Supplementary material

For brevity, we collect some additional simulation and theoretical results, and the proofs of main lemmas, theorems and propositions in the on-line supplementary material.

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References

- Belitser, E. and Ghosal, S. (2003) Adaptive Bayesian inference on the mean of an infinite-dimensional normal distribution. *Ann. Statist.*, **31**, 536–559.
- Brown, L. D., Cai, T. T., Low, M. G. and Zhang, C.-H. (2002) Asymptotic equivalence theory for nonparametric regression with random design. *Ann. Statist.*, **30**, 688–707.
- Brown, L. D. and Levine, M. (2007) Variance estimation on nonparametric regression via the difference sequence method. *Ann. Statist.*, **35**, 2219–2232.
- Brown, L. D. and Low, M. G. (1996) Asymptotic equivalence of nonparametric regression and white noise. *Ann. Statist.*, **24**, 2384–2398.
- Cai, T. T. (1999) Adaptive wavelet estimation: a block thresholding and oracle inequality approach. *Ann. Statist.*, **27**, 898–924.
- Cai, T. T. (2012) Minimax and adaptive inference in nonparametric function estimation. *Statist. Sci.*, **27**, 31–50.
- Cai, T. T. and Yuan, M. (2011) Optimal estimation of the mean function based on discretely sampled functional data: phase transition. *Ann. Statist.*, **39**, 2330–2355.
- Candes, E. J. (2006) Modern statistical estimation via oracle inequalities. *Acta Numer.*, **15**, 1–69.
- Cavalier, L. and Tsybakov, A. (2002) Sharp adaptation for inverse problems with random noise. *Probab. Theory Reltd Flds*, **123**, 323–354.
- Cho, H. (2016) Change-point detection in panel data via double CUSUM statistic. *Electron. J. Statist.*, **10**, 2000–2038.
- Cohen, A. (2003) *Numerical Analysis of Wavelet Methods*, 1st edn. New York: Elsevier.
- Donoho, D. L. (1993) Unconditional bases are optimal bases for data compression and for statistical estimation. *Appl. Computnl Harm. Anal.*, **1**, 100–115.
- Donoho, D. L. and Johnstone, I. M. (1994) Ideal spatial adaption by wavelet shrinkage. *Biometrika*, **81**, 425–455.
- Donoho, D. L., Johnstone, I. M., Kerkycharian, G. and Picard, D. (1995) Wavelet shrinkage: asymptopia (with discussion)? *J. R. Statist. Soc. B*, **57**, 301–369.
- Donoho, D. L., Liu, R. C. and MacGibbon, B. (1990) Minimax risk over hyperrectangles, and implications. *Ann. Statist.*, **18**, 1416–1437.

- Fan, J. and Yao, Q. (1998) Efficient estimation of conditional variance functions in stochastic regression. *Biometrika*, **85**, 645–660.
- Freedman, D. (1999) On the Bernstein-von Mises theorem with infinite-dimensional parameters. *Ann. Statist.*, **27**, 1119–1141.
- Fryzlewicz, P. (2014) Wild binary segmentation for multiple change-point detection. *Ann. Statist.*, **42**, 2243–2281.
- Fryzlewicz, P. (2016) Tail-greedy bottom-up data decompositions and fast multiple change-point detection. Department of Statistics, London School of Economics and Political Science, London. (Available from <http://stats.lse.ac.uk/fryzlewicz/tguh/tguh.pdf>.)
- Hall, P. and Carroll, R. J. (1989) Variance function estimation in regression: the effect of estimating the mean. *J. R. Statist. Soc. B*, **51**, 3–14.
- Hall, P., Kay, J. and Titterton, D. (1990) Asymptotically optimal difference-based estimation of variance in nonparametric regression. *Biometrika*, **77**, 521–528.
- Hall, P. and Marron, J. S. (1990) On variance estimation in nonparametric regression. *Biometrika*, **77**, 415–419.
- Hall, P., Müller, H.-G. and Wang, J.-L. (2006) Properties of principal component methods for functional and longitudinal data analysis. *Ann. Statist.*, **34**, 1493–1517.
- Hastie, T., Buja, A. and Tibshirani, R. (1995) Penalized discriminant analysis. *Ann. Statist.*, **23**, 73–102.
- Johnstone, I. M. (2015) *Gaussian Estimation: Sequence and Multiresolution Models*. Department of Statistics, Stanford University, Stanford. Unpublished.
- Li, Y. and Hsing, T. (2010) Uniform convergence rates for nonparametric regression and principal component analysis in functional/longitudinal data. *Ann. Statist.*, **38**, 3321–3351.
- Mallat, S., Papanicolaou, G. and Zhang, Z. (1998) Adaptive covariance estimation of locally stationary processes. *Ann. Statist.*, **26**, 1–47.
- Müller, H.-G. and Stadtmüller, U. (1987) Estimation of heteroscedasticity in regression analysis. *Ann. Statist.*, **15**, 610–625.
- Pickands, J. (1969) An iterated logarithm law for the maximum in a stationary Gaussian sequence. *Zeits. Wahrsch. Ver. Geb.*, **12**, 344–353.
- Ramsay, J. O. and Silverman, B. W. (2005) *Functional Data Analysis*, 2nd edn. New York: Springer.
- Reiß, M. (2008) Asymptotic equivalence for nonparametric regression with multivariate and random design. *Ann. Statist.*, **36**, 1957–1982.
- Ritter, K. (2000) *Average-case Analysis of Numerical Problems*. Berlin: Springer.
- Ritter, K., Wasilkowski, G. W. and Woźniakowski, H. (1995) Multivariate integration and approximation for random fields satisfying Sacks-Ylvisaker conditions. *Ann. Appl. Probab.*, **5**, 518–540.
- Szabó, B. T., van der Vaart, A. W. and van Zanten, J. H. (2013) Empirical Bayes scaling of Gaussian priors in the white noise model. *Electron. J. Statist.*, **7**, 991–1018.
- Tsybakov, A. B. (2009) *Introduction to Nonparametric Estimation*. New York: Springer.
- Walter, G. G. and Shen, X. (2000) *Wavelets and Other Orthogonal Systems*. Boca Raton: Chapman and Hall–CRC.
- Xiao, L., Zippunikov, V., Ruppert, D. and Crainiceanu, C. (2016) Fast covariance estimation for high-dimensional functional data. *Statist. Comput.*, **26**, 409–421.
- Yao, F., Müller, H.-G. and Wang, J.-L. (2005) Functional data analysis for sparse longitudinal data. *J. Am. Statist. Ass.*, **100**, 577–590.
- Zhang, C.-H. (2005) General empirical Bayes wavelet methods and exactly adaptive minimax estimation. *Ann. Statist.*, **33**, 54–100.
- Zhao, L. H. (2000) Bayesian aspects of some nonparametric problems. *Ann. Statist.*, **28**, 532–552.

Supporting information

Additional ‘supporting information’ may be found in the on-line version of this article:

‘Supplementary material for “From multiple Gaussian sequences to functional data and beyond: a Stein estimation approach”’.