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# Uncertainty Quantification for Stochastic Approximation Limits Using Chaos Expansion\*

S. Crépey<sup>†</sup>, G. Fort<sup>‡</sup>, E. Gobet<sup>§</sup> and U. Stazhynski<sup>¶</sup>

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## Abstract

We analyze the uncertainty quantification for the limit of a stochastic approximation (SA for short) algorithm. Typically, this limit  $\phi^*$  is deterministic and given as the zero of a function written as an expectation. In our setup, the limit  $\phi^*$  is modeled as uncertain through a parameter  $\theta$ . We aim at deriving the probabilistic distribution of  $\phi^*(\theta)$ , given a probability distribution  $\pi$  for  $\theta$ . We introduce an SA algorithm in increasing dimension for computing the basis coefficients of a chaos expansion of  $\phi^*$  on an orthogonal basis of a suitable Hilbert space. The procedure returns a series of estimated coefficients, the corresponding approximation  $\widehat{\phi^*}(\cdot)$  of  $\phi^*(\cdot)$ , and simple approximations of the expectation and variance of  $\{\widehat{\phi^*}(\theta); \theta \sim \pi\}$  (as well as higher order moments when the basis is made of polynomials). The evaluation of more general statistics is possible using  $\widehat{\phi^*}(\cdot)$  and extra i.i.d. Monte-Carlo draws of  $\theta \sim \pi$ . Under explicit assumptions on stochastic approximation limits without uncertainty, we establish

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the almost sure convergence in the Hilbert space of the algorithm.

**KEYWORDS:** stochastic approximation, chaos expansion, uncertainty quantification, stochastic programming, Hilbert space, almost sure convergence, algorithm.

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## 1 Introduction

Since the seminal work of Robbins and Monro [RM51], the method of stochastic approximation (SA for short) has become mainstream for various applications, such as optimization, parameter estimation, signal processing, adaptive control, Monte Carlo optimization of stochastic systems (see [KY97, BMP90]), stochastic gradient descent methods in machine learning (see e.g. [BC05, SSS08, BCN16]), adaptive Monte Carlo sampler (see e.g. [HST01, AT08, FMP11, FJLS16, FS00, DVA98]), and efficient tail computations [BFP09], among others.

Typically, SA is used to find zeros of a function that is only available in the form of an expectation, i.e. for solving equations of the form  $\mathbb{E}[H(z, V)] = 0$ , where  $V$  is some random source of noise. In this work our goal is to study the uncertainty quantification (UQ for short) problem for the stochastic approximation limits (the zeros), denoted by  $\phi^*$ . The field of model uncertainty deals with the situation where the law of the random noise  $V$  is not known exactly. This is expressed in the form of a parametric dependence  $V \sim \mu(\theta, dv)$  where the distribution of  $V$  depends on an unknown parameter  $\theta$  for which only some probability distribution  $\pi$  is available. The uncertainty can also come from the function  $H$ , through a dependency in the uncertain parameter  $\theta$ . Therefore, the equation to solve becomes

$$h(z, \theta) := \int_{\mathcal{V}} H(z, v, \theta) \mu(\theta, dv) = 0, \quad \pi\text{-a.s.}, \quad (1.1)$$

so that the zero  $\phi^*$  depends on  $\theta$ , i.e.  $\phi^* = \phi^*(\theta)$ . For the sake of simplicity in this and the next section, we assume a one-to-one mapping  $\phi^*$  (belonging to a suitable Hilbert space), but in Section 3 our main algorithm is proved to be convergent even in the case of multiple zeros (so that it covers the important VaR/CVaR example, see Remark 3.1).

In this setup the UQ problem consists in determining the distribution of  $\{\phi^*(\theta) : \theta \sim \pi\}$ . Among the possible methodologies reviewed in Section 1.1, we choose the chaos expansion, which consists in computing the coefficients of the function  $\phi^*$  on an orthogonal basis of the  $L^2$  space with respect to the distribution  $\pi$ . The distribution of  $\{\phi^*(\theta) : \theta \sim \pi\}$  can then be approximated by an

empirical distribution, i.e. by sampling independent and identically distributed  $\theta$  and computing our approximation of  $\phi^*$  at the corresponding values of  $\theta$ .

Here, obviously, the most demanding part is the numerical computation of  $\phi^*$ . In this paper, we design an SA algorithm for  $\phi^*$  so that each iteration lies in finite dimensional subspace of the Hilbert space, while the dimension of these subspaces goes to infinity. Like usual SA algorithms, our algorithm is sequential, so that at any iteration it can be stopped and provides a numerical approximation of  $\phi^*$  with some controlled accuracy.

Beyond model uncertainty, applications of our approach include sensitivity analysis, with respect to  $\theta$ , or quasi-regression in the sense of reconstructing a whole unknown function, for instance in the context of nested Monte Carlo computations involving a nonlinear inner function  $\phi^* = \phi^*(\theta)$ . These applications are developed in the companion paper [BCD<sup>+</sup>17].

## 1.1 Literature Background

In UQ applications (see [LK10, Smi14]), the function  $\phi^*$  is typically given as the solution to an auxiliary problem, which requires some numerical computations. Quite often,  $\phi^*$  is solution to a partial differential equation (PDE for short). In our SA setup, the function  $\phi^*$  is given as limits of an SA algorithm parameterized by  $\theta$ .

A first possible approach is based on crude Monte-Carlo (MC) methods, which consist in sampling  $M$  independent and identically distributed  $\theta$  and computing, for each sample  $\theta_m$ ,  $\phi^*(\theta_m)$  or a numerical approximation  $\hat{\phi}^*(\theta_m)$  (in our setting, it would be the output of a standard SA algorithm for fixed  $\theta_m$ , see Section 2.1). The distribution of the random variable  $\{\phi^*(\theta), \theta \sim \pi\}$  is then approximated by the empirical distribution of  $\{\hat{\phi}^*(\theta_m) : 1 \leq m \leq M\}$ . When  $\phi^*$  solves a PDE, a global error analysis is performed in [BTZ04], accounting for both the sampling error and the PDE discretization error, which are decoupled in some way. Our approach is different since we would like to couple in an efficient way the outer sampling of  $\theta$  and the inner simulations used in the SA algorithm.

An alternative method developed in [LBM86, KH92] is a perturbative approach taking advantage of a stochastic expansion of  $\{\phi^*(\theta), \theta \sim \pi\}$  that is available when  $\theta$  has small variations (a restriction that we do not need or want to impose in our case).

**Approximation in  $L^2$ -Spaces.** A third strategy, which dates back to Wiener [Wie38] and has been developed in the fields of engineering and uncertainty quantification in the 2000s (see [GS03, LK10] and references therein), is based on chaos expansions. This technique, also known as the spectral method, consists in projecting the unknown function  $\phi^* : \Theta \mapsto \mathbb{R}^q$  on an orthonormal basis

$\{\theta \mapsto B_i(\theta), i \in \mathbb{N}\}$  of the  $L^2$  space with respect to the distribution  $\pi$ , computing the coefficients of  $\phi = \phi^*$  in its decomposition

$$\phi = \sum_{i \geq 0} u_i B_i. \tag{1.2}$$

In the most common case where  $B_0 \equiv 1$ , once the  $\mathbb{R}^q$ -valued projection coefficients  $\{u_i, i \geq \mathbb{N}\}$  have been computed, the expectation and the variance-covariance matrix are available for free as

$$\mathbb{E}_{\theta \sim \pi}[\phi(\theta)] = u_0 \text{ and } \text{Var}_{\theta \sim \pi}(\phi(\theta)) = \sum_{i \geq 1} u_i u_i^\top.$$

In the case of a polynomial basis, higher order moments are also usually computable explicitly, see [LK10, Appendix C]. This makes this approach potentially much cheaper than the above-mentioned crude MC method.

In the case of an explicitly known function  $\phi$ , finding individual coefficients  $u_i$  is straightforward by MC simulation. But, even then, the global convergence of the method is subject to a nontrivial tuning of the speeds at which the number of coefficients and the number of simulations go to infinity (see [GS14]). In the present paper we deal with the case where the function  $\phi = \phi^*$  is not known explicitly (but only implicitly as the solution to (1.1)), making both the algorithm itself and its convergence analysis more complicated.

In [KB09], the authors provide a finite dimensional procedure to approximate the function  $\phi^*$  minimizing  $\int_{\Theta} L(\phi(\theta), \theta) \pi(d\theta)$ , for some explicitly known function  $L$ , and they analyze the error due to finite dimensional truncation. In our SA setup (1.1), which would correspond to

$$\nabla_z L(z, \theta) = h(z, \theta) \tag{1.3}$$

(cf. (1.1)), restricting the functional space to a finite dimensional subspace would lead to intractable error analysis (cf. Section 2.3). Moreover it requires to choose the dimension in advance, while our approach chooses it adaptively.

### Stochastic Approximation in Hilbert spaces for Statistical Learning.

Recently numerous works have been devoted to statistical learning in Hilbert spaces, in particular, reproducing kernel Hilbert spaces (see e.g. [DB16] and references therein). However, these works cannot be directly related to our problem. First, the setting (typically a regression problem) is different. Second, the loss function in the optimization is usually quadratic plus a penalization term accounting for the regularity of the unknown function. As far as the SA algorithm is concerned, our  $h$  would correspond to the gradient of their loss function (cf. (1.3)). In our study, we consider more general functions  $H$ .

**Stochastic Approximation in Infinite Dimension.** There exists a large number of works on infinite dimensional SA. In [Wal77], [BS89] and [YZ90] the authors study SA in Hilbert spaces in the case of a noise that is independent of the SA iteration, i.e.  $H(z, V) = \tilde{H}(z) + V$ . The conditions of convergence are then similar to those of the finite dimensional case. In [BM13] the authors provide nonasymptotic analysis of SA algorithms in Hilbert spaces with applications to machine learning.

But, although interesting from a theoretical point of view, these SA algorithms are defined directly in the infinite dimensional Hilbert space, so that they are not feasible in practice. By contrast, our SA algorithm works in iteratively increasing dimension (possibly to  $\infty$  in the limit).

There have been already several papers in this direction, generally known as the sieve approach. [Gol88] proves almost-sure convergence in the norm topology for a modified Kiefer-Wolfowitz (see [KW52]) procedure in infinite dimensional Hilbert space using a sieve approach. [Nix84] shows asymptotic normality for a modified sieve-type Robbins-Monro procedure. [Yin92] proves almost-sure convergence in the weak topology for a sieve-type Robbins-Monro procedure. The latter three papers treat the case of independent noise  $H(z, V) = \tilde{H}(z) + V$ , while [CW02] combine the abstract approach [Wal77, BS89, YZ90] with the sieve approach [Nix84, Gol88, Yin92], deriving results on the convergence and asymptotic normality for SA with growing dimension in a quite general setting. However, this literature is insufficient for dealing with uncertainty quantification, for the following reasons:

- Most of the previous papers in a Hilbert space  $\mathcal{H}$  consider a noise term of the form  $\widehat{H}(\phi^k(\cdot), V_{k+1})$  with  $\widehat{H} : \mathcal{H} \times \mathcal{V} \rightarrow \mathcal{H}$ . By contrast, in our case,  $H(\phi^k(\cdot), V_{k+1}, \cdot)$  can only be simulated  $\theta$  by  $\theta$ , as the distribution of  $V_{k+1}$  may depend on  $\theta$  (let alone that simulating “all the  $\theta$  simultaneously” would be computationally too demanding);
- The above-mentioned results are proved under fairly general but at the same time abstract conditions. In an uncertainty quantification framework, we aim at formulating hypotheses in terms of underlying problems corresponding to fixed values of  $\theta$  (without uncertainty). Many of the assumptions in [YZ90] and [CW02] are hard to check, others simply do not hold in our setting (see Remark 3.3);
- Previous works do not discuss implementation details, complexity issues or numerical tests. In various places the actual implementation is unclear. By contrast we provide a fully constructive, easy to implement algorithm.

## 1.2 Contributions and Outline of the Paper

In this paper:

- We design a convergent SA algorithm, of the sieve type, for analyzing the uncertainty quantification of SA limits, in a chaos expansion setup;
- This is a fully constructive, detailed, and easy to implement algorithm (the USA algorithm, Uncertainty for Stochastic Approximation);
- The convergence conditions are explicit hypotheses on finite dimensional problems for fixed values of  $\theta$ , as opposed to abstract assumptions involving Hilbert space notions that are often hard to check in practice;
- We provide extensive reports and discussion on numerical tests.

Section 2 provides a detailed presentation of the problem and introduces three possible algorithms for solving it. Section 3 states the almost sure convergence of the USA algorithm and its  $L^p$  convergence with respect to the underlying Hilbert space norm. The proof is deferred to Section 4. Section 5 presents the results of numerical experiments, including a detailed discussion of the choice of the method parameters.

## 2 Problem Formulations and Algorithmic Solutions

Let  $\mathcal{V}$  be a metric space endowed with its Borel  $\sigma$ -field,  $\Theta$  be a subset of  $\mathbb{R}^d$ , and  $H : \mathbb{R}^q \times \mathcal{V} \times \Theta \rightarrow \mathbb{R}^q$ . Let  $\pi$  be a probability distribution on  $\Theta$  and  $\mu$  be a transition kernel from  $\Theta$  to  $\mathcal{V}$ . We define the scalar product induced by  $\pi$  by

$$\langle f; g \rangle_\pi := \int_{\Theta} f(\theta)g(\theta)\pi(d\theta), \quad (2.1)$$

for any measurable functions  $f, g : \Theta \rightarrow \mathbb{R}$ . By extension, for measurable functions  $f = (f_1, \dots, f_q) : \Theta \rightarrow \mathbb{R}^q$  and  $g : \Theta \rightarrow \mathbb{R}$ , we write in vector form

$$\langle f; g \rangle_\pi := \begin{bmatrix} \langle f_1; g \rangle_\pi \\ \dots \\ \langle f_q; g \rangle_\pi \end{bmatrix}. \quad (2.2)$$

We denote by  $L_{2,q}^\pi$  the Hilbert space of functions  $f : \Theta \rightarrow \mathbb{R}^q$  such that the norm  $\|f\|_\pi := \sqrt{\sum_{i=1}^q \langle f_i; f_i \rangle_\pi}$  is finite.

We consider the following problem:

$$\text{Finding } \phi^* \text{ in } L_{2,q}^\pi \text{ such that } \int_{\mathcal{V}} H(\phi^*(\theta), v, \theta) \mu(\theta, dv) = 0, \quad \pi\text{-a.s.} \quad (2.3)$$

We work on a probability space with expectation denoted by  $\mathbb{E}$ .

## 2.1 SA Approach “ $\theta$ by $\theta$ ”

A naive approach for solving (2.3) is to calculate  $\phi^*(\theta)$  for each value of  $\theta$  separately, for example by the following standard (unparameterized) SA scheme (see [BMP90, Duf97, KY97]): Given a deterministic sequence  $\{\gamma_k, k \in \mathbb{N}\}$  of positive step sizes and a sequence of independent and identically distributed (i.i.d.) r.v.  $\{V_k, k \in \mathbb{N}\}$  sampled from  $\mu(\theta, \cdot)$ , obtain  $\phi^*(\theta)$  as the limit of an iterative scheme

$$\phi^{k+1}(\theta) = \phi^k(\theta) - \gamma_{k+1} H(\phi^k(\theta), V_{k+1}, \theta). \quad (2.4)$$

Explicit conditions can be formulated to the effect that  $\phi^*(\theta) = \lim_k \phi^k(\theta)$  holds on the convergence set of the sequence  $\{\phi^k, k \in \mathbb{N}\}$  (see e.g. [Duf97, Chapter 1]). For  $\lim_k k\gamma_k = O(1)$ , the error  $\mathbb{E}_{\theta \sim \pi} [|\phi^k(\theta) - \phi^*(\theta)|^2]$  after  $k$  iterations (and thus  $k$  Monte Carlo samples) is  $O(1/k)$  (see [Duf97, Chapter 2]).

However, except in the case where  $\Theta$  is finite with few elements, the estimation of  $\phi^*(\theta)$ , separately for each  $\theta \in \Theta$ , is unfeasible (or too demanding computationally).

## 2.2 Chaos Extension Setup and Approach “Coefficient by Coefficient”

Let  $\{\theta \mapsto B_i(\theta), i \in \mathbb{N}\}$  be an orthonormal basis of  $L_{2,1}^\pi$  (for the scalar product (2.1)). Orthonormal polynomials are natural candidates, but there are other possibilities.

**Example 1** (of orthogonal bases). See [CHQZ06, Chapter 2] for the four first examples based on orthogonal polynomials in dimension  $d = 1$ . An orthonormal basis  $\{B_i, i \in \mathbb{N}\}$  can then be obtained by renormalization of the given orthogonal basis.

- (i) If  $\pi(d\theta)$  has the density  $1/(\pi\sqrt{1-\theta^2})$  with respect to the Lebesgue measure on  $\Theta = [-1, 1]$ , then the Chebyshev polynomials of the first kind form an orthogonal basis.
- (ii) If  $\pi(d\theta)$  has the density  $2\sqrt{1-\theta^2}/\pi$  w.r.t. the Lebesgue measure on  $\Theta = [-1, 1]$ , then the Chebyshev polynomials of the second kind form an orthogonal basis.

- (iii) If  $\pi(d\theta)$  is the uniform distribution on the interval  $\Theta = [-1, 1]$ , then the Legendre polynomials form an orthogonal basis.
- (iv) More generally, if  $\pi(d\theta)$  is the distribution on  $[-1, 1]$  with density proportional to  $(1 - \theta)^\alpha(1 + \theta)^\beta$  for some  $\alpha, \beta > -1$ , then the Jacobi polynomials form an orthogonal basis.
- (v) If  $\pi(d\theta)$  is the uniform distribution on the interval  $\Theta = [-\pi, \pi]$ , then we have the orthogonal Fourier basis  $\{1, \cos(i\theta), \sin(i\theta), i \in \mathbb{N}^*\}$ .
- (vi) If  $\{B_i, i \in \mathbb{N}\}$  is an orthogonal basis on  $\Theta \subset \mathbb{R}$  with respect to the distribution  $\pi(d\theta) = \pi(\theta)d\theta$ , then, for any continuously differentiable increasing function  $\varphi$ ,  $\{B_i(\varphi(\cdot)), i \in \mathbb{N}\}$  is an orthogonal basis on  $\varphi^{-1}(\Theta)$  with respect to the distribution  $\pi(\varphi(v))\varphi'(v)dv$ .
- (vii) For a multidimensional distribution ( $d > 1$ ), with independent components, an orthogonal basis is given by the set of all possible products of basis functions of a single variable (see [CHQZ06, Section 5.8]).

For  $x, y \in \mathbb{R}^q$  we denote by  $x \cdot y$  and  $|x|$  the scalar product and the Euclidean norm in  $\mathbb{R}^q$ . We denote by  $l_{2,q}$  the normed vector space of the  $\mathbb{R}^q$ -valued sequences  $\{u_i, i \in \mathbb{N}\}$  with  $\sum_{i \geq 0} |u_i|^2 < +\infty$ . As is well known, given an orthonormal basis  $\{B_i, i \in \mathbb{N}\}$  in  $L_2^\pi$  of  $L_{2,1}^\pi$ , any function  $\phi \in L_{2,q}^\pi$  is characterized by a sequence  $\{u_i, i \in \mathbb{N}\}$  in  $l_{2,q}$  such that  $\phi = \sum_{i \geq 0} u_i B_i$ . Throughout the paper, we use the natural isomorphism  $\mathbf{Is} : l_{2,q} \rightarrow L_{2,q}^\pi$  given by

$$\phi = \mathbf{Is}(u) = \sum_{i \geq 0} u_i B_i, \text{ i.e. } u_i = \langle \phi; B_i \rangle_\pi \text{ for each } i \in \mathbb{N}, \quad (2.5)$$

and the corresponding isometry  $\|\phi\|_\pi = \|u\|_{l_{2,q}}$  (see [Mus14, Proposition 10.32]). In view of this, the problem (2.3) can be restated on  $l_{2,q}$  as

$$\text{Finding } u^* \text{ in } l_{2,q}; \quad \int_{\mathcal{V}} H \left( \sum_{i \geq 0} u_i^* B_i(\theta), v, \theta \right) \mu(\theta, dv) = 0, \quad \pi\text{-a.s.} \quad (2.6)$$

Hence, an alternative strategy for solving (2.3) consists in the estimation of the  $\mathbb{R}^q$ -valued coefficients  $\{u_i^*, i \in \mathbb{N}\}$  of  $\phi^*$ , combined with a truncation at a fixed level  $m$  of the expansion (2.5) and a Monte Carlo approximation of the coefficients  $\{u_i^*, i \leq m\}$ .

Let us discuss the computational cost of this approach, in the case  $q = 1$  for ease of notation (and dimension  $d$  of  $\theta$ ). In the case of a Jacobi polynomial basis,

the following control on the truncation error of  $\phi$  holds (see [Fun92, Theorem 6.4.2] or [CHQZ06, Chapter 5]):

$$\left\| \sum_{i>m} u_i B_i \right\|_{\pi}^2 = O\left(m^{-\frac{2(\eta-1)}{d}}\right), \quad (2.7)$$

where  $\eta$  is the order of continuous differentiability of  $\phi$  (in some cases the order may be strengthened to  $O\left(m^{-\frac{2\eta}{d}}\right)$ ). Furthermore, for  $i \in \mathbb{N}$ , we have

$$u_i = \langle \phi; B_i \rangle_{\pi} \approx \hat{u}_i := \frac{1}{M} \sum_{k=1}^M \widehat{\phi(\theta_{k,i})} B_i(\theta_{k,i}), \quad (2.8)$$

where  $\{\theta_{k,i}, k \in \mathbb{N}, i \leq m\}$  are i.i.d. with distribution  $\pi$  and  $\widehat{\phi(\theta_{k,i})}$  is an approximation of  $\phi(\theta_{k,i})$ . Neglecting the error associated with the approximation  $\widehat{\phi(\theta_{k,i})} \approx \phi(\theta_{k,i})$ , we have

$$\mathbb{E} \left[ \left\| \sum_{i=0}^m (u_i - \hat{u}_i) B_i \right\|_{\pi}^2 \right] = O\left(\frac{m}{M}\right). \quad (2.9)$$

For balancing the error components (2.7) and (2.9), we must set  $M = m^{1+\frac{2(\eta-1)}{d}}$ . To reach a precision  $\epsilon$ ,  $m$  has to increase as  $\epsilon^{-d/(2(\eta-1))}$  and  $M$  has to increase as  $\epsilon^{-(1+d/(2(\eta-1)))}$ . The computational cost in terms of number of Monte Carlo samples to estimate  $m$  coefficients is therefore  $\epsilon^{-(1+d/(\eta-1))}$ . This quantity suffers from the curse of dimensionality, which makes this approach fairly inefficient when combined with a nested procedure for the computation of  $\widehat{\phi(\theta_{k,i})}$ , e.g. through (2.4) if  $\phi = \phi^*$ .

### 2.3 The USA Algorithm

Note that the problem (2.3) is equivalent to finding  $\phi^* \in L_{2,q}^{\pi}$  such that

$$\int_{\Theta} \left( \int_{\mathcal{V}} H(\phi^*(\theta), v, \theta) \mu(\theta, dv) \right) B_i(\theta) \pi(d\theta) = 0_{\mathbb{R}^q}, \quad \forall i \in \mathbb{N}. \quad (2.10)$$

This observation can be used for devising an original SA scheme for the  $u_i^*$  in (2.6).

A first attempt in this direction is to restrict the problem to a set of functions  $\phi$  of the form  $\sum_{i=0}^m u_i B_i$ , for some fixed  $m \in \mathbb{N}$ . If, in addition,  $\mu(\theta, dv) = \mu(dv)$ , and assuming the scalar product  $\langle \cdot; \cdot \rangle_{\pi}$  (corresponding to the integral in

(2.11)) computable exactly (possibly at a large computational cost), then an SA algorithm for the computation of  $\{u_i^*, i \leq m\}$  consists in iterating (cf. [CW02] and the related discussion in the end of Section 1.1):

$$u_i^{k+1} = u_i^k - \gamma_{k+1} \int_{\Theta} H \left( \sum_{j=0}^m u_j^k B_j(\theta), V_{k+1}, \theta \right) B_i(\theta) \pi(d\theta) \quad i = 0, \dots, m, \quad (2.11)$$

where the  $\{(V_k), k \geq 0\}$  are i.i.d. with distribution  $\mu(dv)$  and  $\{\gamma_k, k \in \mathbb{N}\}$  is a deterministic stepsize sequence. In the more general case, an SA algorithm for the computation of  $\{u_i^*, i \leq m\}$  is given by

$$u_i^{k+1} = u_i^k - \gamma_{k+1} H \left( \sum_{j=0}^m u_j^k B_j(\theta_{k+1}), V_{k+1}, \theta_{k+1} \right) B_i(\theta_{k+1}), \quad i = 0, \dots, m, \quad (2.12)$$

where the  $\{(\theta_k, V_k), k \geq 0\}$  are i.i.d. with distribution  $\pi(d\theta)\mu(\theta, dv)$ .

However, in practice, we do not know whether  $\phi^*$  is of the form  $\sum_{i=0}^m u_i B_i$  and, even if so, we may not know for which  $m$ . We emphasize that, in the general case  $\phi^* \in L_{2,q}^\pi$ , as the first argument of  $H$  in (2.12) is the current truncation  $\sum_{i=0}^m u_i^k B_i(\theta_{k+1})$  and not  $\phi^*(\theta_{k+1})$ , this algorithm does not provide the projection of  $\phi^*$  onto the space spanned by  $\{B_0, \dots, B_m\}$ . See the numerical evidence reported in Section 5.4.

Accordingly, the final version of the algorithm tackles the infinite dimensionality of the problem space  $L_{2,q}^\pi$  on which the problem is stated by increasing  $m$ , to recover in the limit the full sequence of the coefficients  $\{u_i^*, i \geq 0\}$  defining a solution  $\phi^* = \sum_i u_i^* B_i$ . Toward this aim, we introduce a sequence  $m_k$  which specifies the number of coefficients  $u_i$  that are updated at the iteration  $k$ . The sequence  $\{m_k, k \geq 0\}$  is nondecreasing and converges to  $\infty$ .

The USA algorithm corresponds to the update of the sequence  $\{u_i^k, i \geq 0\}$  through the following SA scheme, where  $\Pi_{\mathcal{A}}$  denotes the projection on a suitable

convex subset  $\mathcal{A}$  of  $l_{2,q}$ :

**Input:** Sequences  $\{\gamma_k, k \geq 1\}$ ,  $\{m_k, k \geq 1\}$ ,  $\{M_k, k \geq 1\}$ ,  $K \in \mathbb{N}$ ,  $\{u_i^0, i = 0, \dots, m_0\}$ , a convex set  $\mathcal{A} \subseteq l_{2,q}$

**for**  $k = 0$  **to**  $K - 1$ , **do**

sample  $(\theta_{k+1}^s, V_{k+1}^s)$ ,  $s = 1 \dots, M_{k+1}$ , under the distribution  $\pi(d\theta)\mu(\theta, dv)$  for  $i > m_{k+1}$  define  $u_i^k = 0$

**for**  $i = 0$  **to**  $m_{k+1}$ , **do**

$\hat{u}_i^{k+1} = u_i^k - \gamma_{k+1} M_{k+1}^{-1} \sum_{s=1}^{M_{k+1}} H\left(\sum_{j=0}^{m_k} u_j^k B_j(\theta_{k+1}^s), V_{k+1}^s, \theta_{k+1}^s\right) B_i(\theta_{k+1}^s)$

$u^{k+1} = \Pi_{\mathcal{A}}(\hat{u}^{k+1})$

**Output:** The vector  $\{u_i^K, i = 0, \dots, m_K\}$ .

**Algorithm 1:** The USA algorithm for the coefficients of the basis decomposition of  $\phi^*$ .

The inputs of the algorithm are: a positive stepsize sequence  $\{\gamma_k, k \geq 1\}$ ; two integer valued sequences  $\{m_k, k \geq 1\}$  and  $\{M_k, k \geq 1\}$  corresponding to the number of nonnull coefficients in the approximation of  $\phi^*$  and to the number of Monte Carlo draws of the pair  $(\theta, V)$  at each iteration  $k$ ; an initial value  $u_0 \in \mathbb{R}^{m_0}$ ; a total number of iterations  $K$ ; a subset  $\mathcal{A}$  of  $l_{2,q}$  on which to project each newly updated sequence of coefficients.

The output of the algorithm is a sequence  $u^K = \{u_i^K, i \leq m_K\}$  approximating a solution  $u^*$  to the problem (2.6). The corresponding approximation  $\phi^K$  of a solution  $\phi^*$  to the problem (2.3) is then

$$\phi^K := \sum_{i=0}^{m_K} u_i^K B_i. \quad (2.13)$$

**Remark 2.1.** *The motivations for the introduction of the projection set  $\mathcal{A}$  and for the averaging over  $M_k$  draws at step  $k$  are discussed in the respective sections 3.2 and 5.5.3.*

## 3 The USA Algorithm Converges

### 3.1 Assumptions

For simplicity of presentation above, we assumed a one-to-one mapping  $\phi^*$ . However, the USA algorithm is proved below to converge even in the case of multiple zeros. Accordingly, Problem (2.6) is reformulated as

Finding  $u^*$  in  $\mathcal{T}^*$  where

$$\mathcal{T}^* := \left\{ u^* \in l_{2,q}; \quad \int_{\mathcal{V}} H \left( \sum_{i \geq 0} u_i^* B_i(\theta), v, \theta \right) \mu(\theta, dv) = 0, \pi\text{-a.s.} \right\}. \quad (3.1)$$

We do not restrict ourselves to the case of a singleton  $\mathcal{T}^*$ . However, we introduce the following assumption on the target set  $\mathcal{T}^*$  in order to guarantee the existence of a (random) limit point  $\phi^\infty$  of the algorithm in this set:

**H1.** *The set  $\mathcal{T}^*$  is compact and non-empty.*

**Remark 3.1.** *Allowing for multiple limits is quite standard in the SA literature. From the point of view of the application to UQ, it may seem meaningless to quantify the uncertainty of a non-uniquely defined quantity. However, enabling multiple limits appears to be the right setting when some components of the vector-valued function  $\phi^*(\cdot) \in \mathbf{Is}(\mathcal{T}^*)$  are unique and some other are multiple. This encompasses the important case of computing quantiles and average quantiles (cf. [BFP09]) of a (uncertain) distribution: the SA approximation for the quantile component may converge to several limits (especially when the distribution has atoms), while for the average quantile component, the limit is unique.*

**H2.**  *$\{M_k, k \geq 1\}$  and  $\{m_k, k \geq 1\}$  are deterministic sequences of positive integers;  $\{\gamma_k, k \geq 1\}$  is a deterministic sequence of positive real numbers such that, for some  $\kappa > 0$ ,*

$$\sum_{k \geq 1} \gamma_k = +\infty, \quad \sum_{k \geq 1} \gamma_k^{1+\kappa} < +\infty, \quad \sum_{k \geq 1} \gamma_k^2 \frac{Q_{m_k}}{M_k} < +\infty, \quad \sum_{k \geq 1} \gamma_k^{1-\kappa} q_{m_k} < +\infty, \quad (3.2)$$

where the sequences  $\{q_m, m \in \mathbb{N}\}$  and  $\{Q_m, m \in \mathbb{N}\}$  are defined by

$$q_m := \sup_{u^* \in \mathcal{T}^*} \sum_{i > m} |u_i^*|^2, \quad Q_m := \sup_{\theta \in \Theta} \sum_{i \leq m} |B_i(\theta)|^2. \quad (3.3)$$

**Remark 3.2.** *Since  $\mathcal{T}^*$  is compact, we have  $\lim_m q_m = 0$  (cf. the proof of Lemma 2). Assumption H2 requires, in particular, that  $Q_m < +\infty$  for any  $m$ . If  $\Theta$  is bounded, then this is verified for any basis of continuous functions. In the case of polynomial basis, the coefficients  $Q_m$  are related to the Christoffel functions [Nev86].*

**H3.** *For any  $z \in \mathbb{R}^q$ ,*

$$\int_{\Theta \times \mathcal{V}} |H(z, v, \theta)| \mu(\theta, dv) \pi(d\theta) < \infty;$$

For any  $z \in \mathbb{R}^q$  and  $\theta \in \Theta$ ,

$$h(z, \theta) := \int_{\mathcal{V}} H(z, v, \theta) \mu(\theta, dv)$$

exists; For any  $\phi \in L_{2,q}^\pi$ , the mapping  $h(\phi(\cdot), \cdot) : \theta \mapsto h(\phi(\theta), \theta)$  is in  $L_{2,q}^\pi$ ; The mapping  $\phi \mapsto h(\phi(\cdot), \cdot)$  from  $L_{2,q}^\pi$  into itself is continuous.

**H4.** For  $\pi$ -almost every  $\theta$ , for any  $z_\theta, z_\theta^* \in \mathbb{R}^q$  such that  $h(z_\theta, \theta) \neq 0$  and  $h(z_\theta^*, \theta) = 0$ ,

$$(z_\theta - z_\theta^*) \cdot h(z_\theta, \theta) > 0.$$

**Remark 3.3.** Previous works on SA in a Hilbert space  $\mathcal{H}$  typically require an assumption of the type

$$\int_{\Theta} (\phi(\theta) - \phi^*(\theta)) \cdot \hat{h}^n(\phi(\theta), \theta) \pi(d\theta) > 0, \quad \forall \phi \in L_{2,q}^\pi \setminus \mathbf{Is}(\mathcal{T}^*), \phi^* \in \mathbf{Is}(\mathcal{T}^*),$$

for  $n$  large enough, where  $\hat{h}^n(\phi(\cdot), \cdot)$  is the approximation of  $h(\phi(\cdot), \cdot)$  using the first  $n$  elements of a basis of  $\mathcal{H}$ : See e.g. [CW02, Assumption A3P(2)], which only requires the above condition for every  $\phi \neq \phi^*$  in the vector space spanned by the first  $n$  basis functions  $B_i$ . However, even this relaxed assumption does not hold in general in our setting. As a counter-example, one may take any  $\phi^* = \sum_{i \in \mathbb{N}} u_i^* B_i$  with non null coefficients  $u_i^*$ ,  $h(z, \theta) = z - \phi^*(\theta)$ , and  $\phi = \phi^n$  given, for every  $n$ , as the truncation

$$\phi^n := \text{Trunc}_n(\phi^*) = \sum_{i \leq n} u_i^* B_i$$

of order  $n$  of  $\phi^*$ . Then, as  $\text{Trunc}_n(\phi^n - \phi^*) = 0_{L_{2,q}^\pi}$  (by definition of  $\phi^n$ ), we have

$$\int_{\Theta} (\phi^n(\theta) - \phi^*(\theta)) \cdot \hat{h}^n(\phi(\theta), \theta) \pi(d\theta) = \int_{\Theta} (\phi^n(\theta) - \phi^*(\theta)) \cdot \text{Trunc}_n(\phi^n - \phi^*)(\theta) \pi(d\theta) = 0,$$

for every  $n$ .

By contrast, [H4](#) is the standard assumption for SA with fixed  $\theta$ .

**H5.** a) There exists a constant  $C_H$  such that, for any  $z \in \mathbb{R}^q$ ,

$$\sup_{\theta \in \Theta} \int_{\mathcal{V}} |H(z, v, \theta)|^2 \mu(\theta, dv) \leq C_H (1 + |z|^2).$$

b) The map from  $L_{2,q}^\pi$  into  $\mathbb{R}$  defined by  $\phi \mapsto \int_{\mathcal{V} \times \Theta} |H(\phi(\theta), v, \theta)|^2 \pi(d\theta) \mu(\theta, dv)$  is bounded, i.e. it maps bounded sets into bounded sets.

Note that [H5-b](#) implies that  $\phi \mapsto h(\phi(\cdot), \cdot)$  is a bounded map from  $L_{2,q}^\pi$  into itself.

**H6.** For any  $B > 0$ , there exists a constant  $C_B > 0$  such that, for any  $(\phi, \phi^*) \in L_{2,q}^\pi \times \mathbf{Is}(\mathcal{T}^*)$  with  $\|\phi - \phi^*\|_\pi \leq B$ ,

$$\int (\phi - \phi^*)(\theta) \cdot h(\phi(\theta), \theta) \pi(d\theta) \geq C_B \min_{\bar{\phi} \in \mathbf{Is}(\mathcal{T}^*)} \|\phi - \bar{\phi}\|_\pi^2.$$

Note that the above minimum exists since  $\mathbf{Is}(\mathcal{T}^*)$  is compact, by [H1](#).

## 3.2 Projection Set

We address the convergence of the algorithm 1 for three possible choices regarding the projection set  $\mathcal{A}$  (which always includes  $\mathcal{T}^*$ ).

**Case 1.**  $\mathcal{A} := l_{2,q}$ .

**Case 2.**  $\mathcal{A}$  is a closed ball of  $l_{2,q}$  containing  $\mathcal{T}^*$ .

**Case 3.**  $\mathcal{A}$  is a closed convex set of  $l_{2,q}$  containing  $\mathcal{T}^*$ , with compact intersections to closed balls of  $l_{2,q}$ .

Note that the projection set  $\mathcal{A}$  is bounded in Case 2 and unbounded in the two other cases (for sure in Case 1 and potentially in 3).

Case 1 is the most convenient from the algorithmic viewpoint since no actual projection is required. However, it requires a stronger condition H5-a to ensure the stability and an additional assumption H6 for the convergence.

The projection on a ball  $\{u \in l_{2,q} : \|u\|_{l_{2,q}} \leq B\}$  is given simply by

$$u \mapsto \min \left( 1, \frac{B}{\|u\|_{l_{2,q}}} \right) u. \quad (3.4)$$

Hence, the projection required in Case 2 is quite straightforward. The milder assumption H5-b is required for the stability but one still needs H6 for the convergence.

Case 3 requires a potentially nontrivial projection on a closed convex set: see e.g. Example 2 below. The stronger condition H5-a is required for both the stability and the convergence, but H6 is not needed.

We now give an example of the set  $\mathcal{A}$  in Case 3.

**Example 2.** Given a positive sequence  $\{a_n, n \in \mathbb{N}\}$  such that  $\sum_{i \geq 0} a_i^2 < \infty$  and an increasing sequence of non-negative integers  $\{d_n, n \in \mathbb{N}\}$ , define the closed convex set  $\mathcal{A}$ :

$$\mathcal{A} := \left\{ u \in l_{2,q} : \sum_{d_n \leq i < d_{n+1}} |u_i|^2 \leq a_n^2 \quad \forall n \in \mathbb{N} \right\}. \quad (3.5)$$

When  $d_0 = 0$ , the set  $\mathcal{A}$  is a compact convex subset of  $l_{2,q}$  (see Lemma 2). Otherwise, it is not necessarily compact. However, the set  $\mathcal{A} \cap \{u \in l_{2,q} : \sum_{i \geq 0} u_i^2 \leq B\}$  is a compact subset for any  $B > 0$  (see Corollary 2). The orthogonal projection on  $\mathcal{A}$  consists in projecting  $(u_{d_n}, \dots, u_{d_{n+1}-1})$  on the ball of radius  $a_n$  for all  $n \in \mathbb{N}$ .

### 3.3 Main Result

**Theorem 1.** *Assume [H1](#) to [H4](#) and [H5-a](#) if  $\mathcal{A}$  is unbounded or [H5-b](#) if  $\mathcal{A}$  is bounded. Let there be given i.i.d. random variables  $\{(\theta_k^s, V_k^s), 1 \leq s \leq M_k, k \geq 1\}$  with distribution  $\pi(d\theta)\mu(\theta, dv)$ . Let  $u^K$  and  $\phi^K$  be the outputs of the USA Algorithm (cf. [\(2.13\)](#)).*

*Stability. For any  $\phi^* \in \mathbf{Is}(\mathcal{T}^*)$ ,  $\lim_{k \rightarrow +\infty} \|\phi^k - \phi^*\|_\pi$  exists, is finite a.s., and we have*

$$\sup_{k \geq 0} \mathbb{E} \left[ \|\phi^k - \phi^*\|_\pi^2 \right] < +\infty. \quad (3.6)$$

*Convergence. In addition, in case [3](#), and in cases [1](#) and [2](#) under the additional assumption [H6](#), there exists a random variable  $\phi^\infty$  taking values in  $\mathbf{Is}(\mathcal{T}^*)$  such that*

$$\lim_{k \rightarrow \infty} \|\phi^k - \phi^\infty\|_\pi = 0 \text{ a.s. and, for any } p \in (0, 2), \lim_{k \rightarrow \infty} \mathbb{E} \left[ \|\phi^k - \phi^\infty\|_\pi^p \right] = 0. \quad (3.7)$$

**Remark 3.4.** *The standard assumption ensuring a central limit theorem (CLT) for SA algorithms in a Hilbert space (cf. [[CW02](#), Assumption B3(1)] or [[Nix84](#), Section 3, equation 3.3]) is not satisfied in our setup: as a counter-example, one can take any polynomial basis and a function  $h(z, \theta)$  such that  $\partial_z h(\phi^*(\theta), \theta) = \theta$ , due to the recurrence relations of order two that are intrinsic to such bases. The study of convergence rates and CLT for the USA algorithm is therefore a problem per se, which we leave for future research.*

## 4 Proof of Theorem 1

Throughout the proof, we will use the notation

$$\phi^k := \sum_{i \geq 0} u_i^k B_i = \sum_{i=0}^{m_k} u_i^k B_i$$

(recalling that  $u_i^k = 0$  for any  $i > m_k$  in the USA Algorithm). For any  $z = (z_1, \dots, z_q) \in \mathbb{R}^q$  and any real-valued sequence  $p := \{p_i, i \geq 0\}$  such that  $\sum_{i \geq 0} p_i^2 < \infty$  we write

$$z \otimes p := ((z_1 p_0, \dots, z_q p_0), (z_1 p_1, \dots, z_q p_1), \dots) \in l_{2,q}.$$

Set  $\mathbf{B}^m(\theta) := (B_0(\theta), \dots, B_m(\theta), 0, 0, \dots)$ . Define the filtration

$$\mathcal{F}_k := \sigma(\theta_\ell^s, V_\ell^s, 1 \leq s \leq M_\ell, 1 \leq \ell \leq k), k \in \mathbb{N}.$$

**We fix  $u^* \in \mathcal{T}^*$ , which exists by [H1](#), and we set  $\phi^* := \mathbf{Is}(u^*)$ .**

## 4.1 Stability

The first step is to prove that the algorithm is stable in the sense that

$$\lim_k \|u^k - u^*\|_{l_{2,q}} \text{ exists a.s. ,} \quad (4.1)$$

$$\sup_k \mathbb{E} \left[ \|u^k - u^*\|_{l_{2,q}}^2 \right] < +\infty, \quad (4.2)$$

$$\liminf_{k \rightarrow \infty} \int_{\Theta} (\phi^k(\theta) - \phi^*(\theta)) \cdot h(\phi^k(\theta), \theta) \pi(d\theta) = 0, \quad \text{a.s.} \quad (4.3)$$

Using the definition of  $u^{k+1}$  in the USA algorithm and the property  $\Pi_{\mathcal{A}}(u^*) = u^*$ , we obtain (recalling that, in all cases 1 to 3,  $\mathcal{T}^* \subseteq \mathcal{A}$ )

$$\begin{aligned} \|\phi^{k+1} - \phi^*\|_{\pi}^2 &= \|u^{k+1} - u^*\|_{l_{2,q}}^2 = \|\Pi_{\mathcal{A}}(\hat{u}^{k+1}) - \Pi_{\mathcal{A}}(u^*)\|_{l_{2,q}}^2 \leq \|\hat{u}^{k+1} - u^*\|_{l_{2,q}}^2 \\ &= \|u^k - u^* - \gamma_{k+1} \mathcal{H}^k - \gamma_{k+1} \eta^{k+1}\|_{l_{2,q}}^2, \end{aligned}$$

where

$$\begin{aligned} \mathcal{H}^k &:= \mathbb{E} \left[ \frac{1}{M_{k+1}} \sum_{s=1}^{M_{k+1}} H(\phi^k(\theta_{k+1}^s), V_{k+1}^s, \theta_{k+1}^s) \otimes \mathbf{B}^{m_{k+1}}(\theta_{k+1}^s) \middle| \mathcal{F}_k \right] \\ &= \int_{\Theta \times \mathcal{V}} H(\phi^k(\theta), v, \theta) \otimes \mathbf{B}^{m_{k+1}}(\theta) \pi(d\theta) \mu(\theta, dv) \\ &= \int_{\Theta} h(\phi^k(\theta), \theta) \otimes \mathbf{B}^{m_{k+1}}(\theta) \pi(d\theta), \\ \eta^{k+1} &:= \frac{1}{M_{k+1}} \sum_{s=1}^{M_{k+1}} H(\phi^k(\theta_{k+1}^s), V_{k+1}^s, \theta_{k+1}^s) \otimes \mathbf{B}^{m_{k+1}}(\theta_{k+1}^s) - \mathcal{H}^k. \end{aligned}$$

For the equivalent definitions of  $\mathcal{H}^k$ , we used the Fubini theorem and [H3](#). Observe that, by definition of  $\mathbf{B}^{m_k}$ ,  $\mathcal{H}^k$  and  $\eta^{k+1}$  are sequences in  $l_{2,q}$  such that, for all  $i > m_{k+1}$ ,

$$\mathcal{H}_i^k = 0_{\mathbb{R}^q}, \quad \eta_i^{k+1} = 0_{\mathbb{R}^q}.$$

Define

$$\bar{\mathcal{H}}_i^k := \begin{cases} \mathcal{H}_i^k & i \leq m_{k+1}, \\ \int_{\Theta} h(\phi^k(\theta), \theta) B_i(\theta) \pi(d\theta) & i > m_{k+1}. \end{cases}$$

Recalling that  $u_i^k = 0_{\mathbb{R}^q}$  for  $i > m_{k+1}$ , we obtain

$$\begin{aligned}
\|u^{k+1} - u^*\|_{l_{2,q}}^2 &= \|u^k - u^*\|_{l_{2,q}}^2 - 2\gamma_{k+1} \sum_{i=0}^{m_{k+1}} (u_i^k - u_i^*) \cdot \mathcal{H}_i^k \\
&\quad - 2\gamma_{k+1} \sum_{i=0}^{m_{k+1}} (u_i^k - u_i^*) \cdot \eta_i^{k+1} \\
&\quad + 2\gamma_{k+1}^2 \sum_{i=0}^{m_{k+1}} \eta_i^{k+1} \cdot \mathcal{H}_i^k + \gamma_{k+1}^2 \|\eta^{k+1}\|_{l_{2,q}}^2 + \gamma_{k+1}^2 \|\mathcal{H}^k\|_{l_{2,q}}^2 \\
&= \|u^k - u^*\|_{l_{2,q}}^2 - 2\gamma_{k+1} \sum_{i \geq 0} (u_i^k - u_i^*) \cdot \overline{\mathcal{H}}_i^k \\
&\quad + 2\gamma_{k+1}^2 \sum_{i=0}^{m_{k+1}} \eta_i^{k+1} \cdot \mathcal{H}_i^k - 2\gamma_{k+1} \sum_{i=0}^{m_{k+1}} (u_i^k - u_i^*) \cdot \eta_i^{k+1} \\
&\quad - 2\gamma_{k+1} \sum_{i > m_{k+1}} u_i^* \cdot \overline{\mathcal{H}}_i^k + \gamma_{k+1}^2 \|\eta^{k+1}\|_{l_{2,q}}^2 + \gamma_{k+1}^2 \|\mathcal{H}^k\|_{l_{2,q}}^2. \quad (4.4)
\end{aligned}$$

H4 implies that, for each  $\theta$ ,

$$\sum_{i \geq 0} ((u_i^k - u_i^*) \cdot h(\phi^k(\theta), \theta)) B_i(\theta) = (\phi^k(\theta) - \phi^*(\theta)) \cdot h(\phi^k(\theta), \theta) \geq 0.$$

Taking expectation with respect to  $\theta \sim \pi$  and applying the Fubini theorem (which follows from H3), we obtain for all  $k \geq 0$

$$L^k := \int_{\Theta} (\phi^k(\theta) - \phi^*(\theta)) \cdot h(\phi^k(\theta), \theta) d\theta = \sum_{i \geq 0} (u_i^k - u_i^*) \cdot \overline{\mathcal{H}}_i^k \geq 0. \quad (4.5)$$

Note also that  $\sum_{i=0}^{+\infty} (u_i^k - u_i^*) \cdot \mathcal{H}_i^k \in \mathcal{F}_k$ . By definition,  $\mathbb{E}[\eta_i^{k+1} | \mathcal{F}_k] = 0$ , so that

$$\mathbb{E} \left[ \sum_{i=0}^{m_{k+1}} \eta_i^{k+1} \cdot \mathcal{H}_i^k \middle| \mathcal{F}_k \right] = 0, \quad \mathbb{E} \left[ \sum_{i=0}^{m_{k+1}} (u_i^k - u_i^*) \cdot \eta_i^{k+1} \middle| \mathcal{F}_k \right] = 0. \quad (4.6)$$

Let us consider the term  $\|\eta^{k+1}\|_{l_{2,q}}^2$ . We write

$$\begin{aligned}
& \mathbb{E} \left[ \|\eta^{k+1}\|_{l_{2,q}}^2 \mid \mathcal{F}_k \right] \\
& \leq \mathbb{E} \left[ \left\| \frac{1}{M_{k+1}} \sum_{s=1}^{M_{k+1}} H(\phi^k(\theta_{k+1}^s), V_{k+1}^s, \theta_{k+1}^s) \otimes \mathbf{B}^{m_{k+1}}(\theta_{k+1}^s) - \mathcal{H}^k \right\|_{l_{2,q}}^2 \mid \mathcal{F}_k \right] \\
& \leq \frac{1}{M_{k+1}} \int_{\Theta \times \mathcal{V}} \|H(\phi^k(\theta), v, \theta) \otimes \mathbf{B}^{m_{k+1}}(\theta)\|_{l_{2,q}}^2 \pi(d\theta) \mu(\theta, dv) \\
& = \frac{1}{M_{k+1}} \int_{\Theta \times \mathcal{V}} |H(\phi^k(\theta), v, \theta)|^2 \left( \sum_{i=0}^{m_{k+1}} B_i(\theta)^2 \right) \pi(d\theta) \mu(\theta, dv) \\
& \leq \frac{Q_{m_{k+1}}}{M_{k+1}} \int_{\Theta \times \mathcal{V}} |H(\phi^k(\theta), v, \theta)|^2 \pi(d\theta) \mu(\theta, dv). \tag{4.7}
\end{aligned}$$

Next we consider the term  $2\gamma_{k+1} \sum_{i>m_{k+1}} u_i^* \cdot \overline{\mathcal{H}}_i^k$ . By using  $2ab \leq a^2 + b^2$  with  $a \leftarrow (\gamma_{k+1}^{1-\kappa})^{1/2} |u_i^*|$  and  $b \leftarrow (\gamma_{k+1}^{1+\kappa})^{1/2} |\overline{\mathcal{H}}_i^k|$ , we have

$$\begin{aligned}
\left| 2\gamma_{k+1} \sum_{i>m_{k+1}} u_i^* \cdot \overline{\mathcal{H}}_i^k \right| & \leq \gamma_{k+1}^{1-\kappa} \left( \sum_{i>m_{k+1}} |u_i^*|^2 \right) + \gamma_{k+1}^{1+\kappa} \left( \sum_{i>m_{k+1}} |\overline{\mathcal{H}}_i^k|^2 \right) \\
& \leq \gamma_{k+1}^{1-\kappa} q_{m_{k+1}} + \gamma_{k+1}^{1+\kappa} \|\overline{\mathcal{H}}^k\|_{l_{2,q}}^2, \tag{4.8}
\end{aligned}$$

where we used [H2](#) in the last inequality. Note that

$$\begin{aligned}
\|\overline{\mathcal{H}}^k\|_{l_{2,q}}^2 & = \sum_{i=0}^{+\infty} \left| \int_{\Theta} h(\phi^k(\theta), \theta) B_i(\theta) \pi(d\theta) \right|^2 = \int_{\Theta} |h(\phi^k(\theta), \theta)|^2 \pi(d\theta) \\
& \leq \int_{\Theta \times \mathcal{V}} |H(\phi^k(\theta), v, \theta)|^2 \pi(d\theta) \mu(\theta, dv). \tag{4.9}
\end{aligned}$$

Combining [\(4.4\)](#), [\(4.5\)](#), [\(4.6\)](#), [\(4.7\)](#), [\(4.8\)](#), and [\(4.9\)](#), we obtain

$$\begin{aligned}
& \mathbb{E} \left[ \|u^{k+1} - u^*\|_{l_{2,q}}^2 \mid \mathcal{F}_k \right] \\
& \leq \|u^k - u^*\|_{l_{2,q}}^2 - 2\gamma_{k+1} L^k + \gamma_{k+1}^{1-\kappa} q_{m_{k+1}} \\
& \quad + \left( \gamma_{k+1}^2 + \gamma_{k+1}^{1+\kappa} + \gamma_{k+1}^2 \frac{Q_{m_{k+1}}}{M_{k+1}} \right) \int_{\Theta \times \mathcal{V}} |H(\phi^k(\theta), v, \theta)|^2 \pi(d\theta) \mu(\theta, dv). \tag{4.10}
\end{aligned}$$

To control the integral in [\(4.10\)](#), we distinguish two cases.

First case:  $\mathcal{A}$  is unbounded. Using H5-a we write

$$\begin{aligned} \int_{\Theta \times \mathcal{V}} |H(\phi^k(\theta), v, \theta)|^2 \pi(d\theta) \mu(\theta, dv) &\leq C_H \int_{\Theta} (1 + |\phi^k(\theta)|^2) \pi(d\theta) \\ &\leq C_1 (1 + \|u^k - u^*\|_{l_{2,q}}^2), \end{aligned}$$

where  $C_1 := 2C_H(1 + \sup_{u^* \in \mathcal{T}^*} \|u^*\|_{l_{2,q}}^2)$ . Note that  $C_1$  is finite by H1.

Second case:  $\mathcal{A}$  is bounded. Note that, by definition of  $u^k$ , there exists a constant  $B$  such that a.s.  $\sup_{k \geq 0} \|u^k\|_{l_{2,q}} \leq B$ . Assumption H5-b implies that, for some finite and positive  $C_2$ ,

$$\sup_{k \geq 0} \int_{\mathcal{V} \times \Theta} |H(\phi^k(\theta), v, \theta)|^2 \pi(d\theta) \mu(\theta, dv) \leq C_2.$$

In either case, we deduce from (4.10) that

$$\begin{aligned} \mathbb{E} \left[ \|u^{k+1} - u^*\|_{l_{2,q}}^2 | \mathcal{F}_k \right] &\leq \|u^k - u^*\|_{l_{2,q}}^2 - 2\gamma_{k+1} L^k + \gamma_{k+1}^{1-\kappa} q_{m_{k+1}} \\ &+ \left( \gamma_{k+1}^2 + \gamma_{k+1}^{1+\kappa} + \gamma_{k+1}^2 \frac{Q_{m_{k+1}}}{M_{k+1}} \right) (C_1 \vee C_2) (1 + \|u^k - u^*\|_{l_{2,q}}^2). \end{aligned} \quad (4.11)$$

**Conclusion.** In view of the above controls and of H2, the assumptions of the Robbins-Siegmund lemma are verified (see [RS71]). An application of this lemma yields that  $\lim_k \|u^k - u^*\|_{l_{2,q}}^2$  exists and  $\sum_{k \geq 0} \gamma_{k+1} L^k < +\infty$  a.s.. This concludes the proof of (4.1). Taking expectations in (4.11) and applying the Robbins-Siegmund lemma to the sequence  $\mathbb{E} \left[ \|u^k - u^*\|_{l_{2,q}}^2 \right]$  yields (4.2). Note also that

$$L := \liminf_{k \rightarrow +\infty} L^k = 0, \quad \text{a.s.} \quad (4.12)$$

Indeed, on the event  $\{L > 0\}$ , there exists a finite random index  $K$  such that  $L^k > L/2$  holds for any  $k \geq K$ , which implies that  $\sum_{k \geq 0} \gamma_{k+1} L^k < +\infty$  (as, by assumption,  $\sum_{k \geq 1} \gamma_k = +\infty$ ). Therefore  $\{L > 0\} \subseteq \{\sum_{k \geq 0} \gamma_{k+1} L^k < +\infty\}$ , where we saw above that  $\{\sum_{k \geq 0} \gamma_{k+1} L^k < +\infty\}$  is a zero probability event. Hence so is  $\{L > 0\}$ , which proves (4.3).

We know from (4.1) that  $\lim_k \|\phi^k - \phi'\|_{\pi}$  exists a.s. for any  $\phi' \in \mathbf{Is}(\mathcal{T}^*)$ . For later use we need the existence of this limit simultaneously for all  $\phi' \in \mathbf{Is}(\mathcal{T}^*)$  with probability one. Note that  $\lim_k \|\phi^k - \phi'\|_{\pi}$  is continuous in  $\phi'$  (by triangle inequality). Using that  $\mathbf{Is}(\mathcal{T}^*)$  is separable as a subset of a separable Hilbert space  $L_{2,q}^{\pi}$ , we deduce that

$$\lim_k \|\phi^k - \phi'\|_{\pi} \text{ exists for all } \phi' \in \mathbf{Is}(\mathcal{T}^*), \quad \text{a.s.} \quad (4.13)$$

## 4.2 Proof of the Almost Sure Convergence in (3.7)

**Proof for Case 1 or Case 2.** Under the assumption H1,  $\mathbf{Is}(\mathcal{T}^*)$  is bounded so that, by (4.1), the random variable  $B := \sup_{\phi^* \in \mathcal{T}^*} \sup_k \|\phi^k - \phi^*\|_\pi$  is finite with probability one. Since by (4.12)  $\liminf_k L^k = 0$ , with probability one, there exists a subsequence  $\{\zeta(k), k \geq 1\}$  such that  $\lim_k L^{\zeta(k)} = 0$ .

From (4.5) and by H6 applied with  $\phi \leftarrow \phi^{\zeta(k)}$  and  $\phi^* \leftarrow \mathbf{Is}(u^*)$ , there exists a positive random variable  $C_B$  (finite a.s. and independent of  $k$  by definition of the r.v.  $B$ ) such that

$$L^{\zeta(k)} \geq C_B \min_{\bar{\phi} \in \mathbf{Is}(\mathcal{T}^*)} \|\phi^{\zeta(k)} - \bar{\phi}\|_\pi^2.$$

Let  $\{\bar{\phi}^k, k \geq 0\}$  be an  $\mathbf{Is}(\mathcal{T}^*)$ -valued sequence such that, for all  $k$ ,

$$\min_{\bar{\phi} \in \mathbf{Is}(\mathcal{T}^*)} \|\phi^{\zeta(k)} - \bar{\phi}\|_\pi^2 = \|\phi^{\zeta(k)} - \bar{\phi}^k\|_\pi^2.$$

Such a sequence exists since  $\mathcal{T}^*$  is compact by H1. Using that  $\lim_k L^{\zeta(k)} = 0$  we obtain  $\lim_k \|\phi^{\zeta(k)} - \bar{\phi}^k\|_\pi = 0$  a.s.. Since the sequence  $\{\bar{\phi}^k, k \geq 0\}$  is in a compact set  $\mathbf{Is}(\mathcal{T}^*)$  (see H1), up to extraction of a subsequence it converges to a random limit  $\phi^\infty \in \mathbf{Is}(\mathcal{T}^*)$ . Hence

$$\lim_k \|\phi^{\zeta(k)} - \phi^\infty\|_\pi = 0 \text{ a.s..}$$

In view of (4.13), we deduce

$$\lim_k \|\phi^k - \phi^\infty\|_\pi = \lim_k \|\phi^{\zeta(k)} - \phi^\infty\|_\pi = 0 \text{ a.s..}$$

This concludes the proof of (3.7).

**Proof for Case 3.** Since by (4.12)  $\liminf_k L^k = 0$  with probability one, there exists a (random) subsequence  $\{\zeta(k), k \geq 1\}$  such that  $\lim_k L^{\zeta(k)} = 0$  a.s. Since the sequence  $\{u^{\zeta(k)}, k \geq 0\}$  is bounded in  $l_{2,q}$  a.s. (as  $\lim_k \|u^k - u^*\|_{l_{2,q}}$  exists a.s.) and belongs to the convex set  $\mathcal{A}$  by construction, hence it belongs to a compact set (see Corollary 2). Therefore we can assume (up to extraction of another subsequence) the existence of  $u^\infty \in L_{2,q}^\pi$  such that  $\lim_k \|u^{\zeta(k)} - u^\infty\|_{l_{2,q}} = 0$  a.s. We now prove that  $u^\infty$  is a  $\mathcal{T}^*$ -valued random variable (possibly depending on the choice of  $u^* \in \mathcal{T}^*$ ). Set  $\phi^\infty := \mathbf{Is}(u^\infty)$  and define

$$L^\infty := \int_{\Theta} (\phi^\infty - \phi^*) (\theta) \cdot h(\phi^\infty(\theta), \theta) \pi(d\theta).$$

Then for any  $j \geq 1$ ,

$$\begin{aligned} L^j - L^\infty &= \int_{\Theta} (\phi^j - \phi^\infty)(\theta) \cdot h(\phi^j(\theta), \theta) \pi(d\theta) \\ &\quad + \int_{\Theta} (\phi^\infty - \phi^*)(\theta) \cdot (h(\phi^j(\theta), \theta) - h(\phi^\infty(\theta), \theta)) \pi(d\theta). \end{aligned}$$

By either [H5-b](#) or [H5-a](#) (depending on whether  $\mathcal{A}$  is bounded or not) and since  $\sup_k \|u^k\|_{l_{2,q}} < \infty$  a.s., we have  $\sup_k \|h(\phi^{\zeta(k)}(\cdot), \cdot)\|_\pi^2 < \infty$  a.s.. Since

$$\lim_k \|\phi^{\zeta(k)} - \phi^\infty\|_\pi = \lim_k \|u^{\zeta(k)} - u^\infty\|_{l_{2,q}} = 0, \quad \text{a.s.},$$

hence

$$\lim_k \int_{\Theta} (\phi^{\zeta(k)} - \phi^\infty)(\theta) \cdot h(\phi^{\zeta(k)}(\theta), \theta) \pi(d\theta) = 0, \quad \text{a.s.}$$

Furthermore, since, by [H3](#),  $\phi \mapsto h(\phi(\cdot), \cdot)$  is continuous in  $L_{2,q}^\pi$ , we have

$$\lim_k \int_{\Theta} (\phi^\infty - \phi^*)(\theta) \cdot (h(\phi^{\zeta(k)}(\theta), \theta) - h(\phi^\infty(\theta), \theta)) \pi(d\theta) = 0 \text{ a.s.}$$

Hence  $0 = \lim_k L^{\zeta(k)} = L^\infty$  a.s. In view of the definition of  $L^\infty$  and of [H4](#), we deduce that  $u^\infty \in \mathcal{T}^*$  a.s.. In view of [\(4.13\)](#), this implies that  $\lim_k \|\phi^k - \phi^\infty\|_\pi = \lim_k \|\phi^{\zeta(k)} - \phi^\infty\|_\pi = 0$ .

### 4.3 Proof of the $L^2$ -Control [\(3.6\)](#) and of the $L^p$ -Convergence in [\(3.7\)](#)

The  $L^2$ -control

$$\sup_{k \geq 0} \mathbb{E} \left[ \|\phi^k - \phi^\infty\|_\pi^2 \right] < +\infty$$

follows directly from [\(4.2\)](#) and the boundedness of  $\mathcal{T}^*$  (see [H1](#)). This proves [\(3.6\)](#).

Let  $C > 0$  and  $p \in (0, 2)$ . We write

$$\mathbb{E} \left[ \|\phi^k - \phi^\infty\|_\pi^p \right] = \mathbb{E} \left[ \|\phi^k - \phi^\infty\|_\pi^p \mathbf{1}_{\{\|\phi^k - \phi^\infty\|_\pi > C\}} \right] + \mathbb{E} \left[ \|\phi^k - \phi^\infty\|_\pi^p \mathbf{1}_{\{\|\phi^k - \phi^\infty\|_\pi \leq C\}} \right].$$

The first term on the right hand side converges to 0 as  $C \rightarrow +\infty$ , uniformly in  $k$ : indeed, we have

$$\mathbb{E} \left[ \|\phi^k - \phi^\infty\|_\pi^p \mathbf{1}_{\{\|\phi^k - \phi^\infty\|_\pi > C\}} \right] \leq \frac{\sup_{l \geq 0} \mathbb{E} \left[ \|\phi^l - \phi^\infty\|_\pi^2 \right]}{C^{2-p}}.$$

For any fixed  $C > 0$ , the second term converges to zero by the dominated convergence theorem. This concludes the proof of [Theorem 1](#).  $\square$

## 5 Numerical Investigations

In this section, we discuss the parameterization of the USA algorithm and we test empirically the sensitivity of its performance with respect to its parameters. Notably, the possibility of letting the number  $m_k$  of estimated coefficients  $u_i^*$  tend to infinity appears not only as a necessary ingredient for proving the theoretical convergence (see Theorem 1), but also as a key feature for its numerical performance, even regarding the estimation of the lower order coefficients  $u_i^*$ . We illustrate this assertion numerically, by testing both the genuine USA algorithm with increasing  $m_k$  and the fixed dimension version with  $m_k = m$  (for different values of  $m$ ), respectively referred to as the “increasing  $m_k$ ” and the “fixed  $m$ ” algorithms henceforth.

There cannot be any comparison, performance-wise, between the USA algorithm and the naive algorithms of Sections 2.1 and 2.2. The “ $\theta$  by  $\theta$ ” algorithm of Section 2.1 is of course no option unless a finite set  $\Theta$ , with reasonable cardinality, is considered. As for the “coefficient by coefficient” algorithm of Section 2.2, it requires one (standard, admittedly) SA algorithm for each estimate  $\widehat{\phi(\theta_{k,i})}$  of  $\phi(\theta_{k,i})$  in (2.8): since  $k$  indexes Monte Carlo draws, it means a nested Monte Carlo approach, which can only be achieved, on realistic applications, by resorting to concurrent computing resources. Instead, the USA algorithm is a single SA procedure (in increasing space dimension) for the joint estimation of the coefficients  $u_i^*$ .

### 5.1 Design Parameterization of the USA Algorithm

When running the USA algorithm, the user has to choose some design parameters: given a problem of the form (3.1) and the corresponding sequence  $\{q_m, m \in \mathbb{N}\}$  via (3.2), the user has to choose the orthogonal basis  $\{B_i(\theta), i \in \mathbb{N}\}$ , which fixes in turn the sequence  $\{Q_m, m \in \mathbb{N}\}$ . It remains to choose  $\{\gamma_k, k \in \mathbb{N}\}$ ,  $\{m_k, k \in \mathbb{N}\}$  and  $\{M_k, k \in \mathbb{N}\}$ . In this section, we consider sequences of the form

$$\gamma_k = k^{-a}, \quad m_k = \lfloor k^b \rfloor + 1, \quad M_k = \lfloor k^p \rfloor + 1, \quad (5.1)$$

for  $a, p \geq 0$  and  $b > 0$ , and we discuss how to choose these constants assuming that

$$q_m = O(m^{-\delta}), \quad Q_m = O(m^L), \quad (5.2)$$

for some  $\delta > 0$  and  $L \geq 0$ .

An easy calculation shows that H2 is satisfied ( $\kappa > 0$  ensuring H2 exists) if

$$0 < a \leq 1, \quad 2 - \delta b < 2a, \quad bL + 1 < 2a + p. \quad (5.3)$$

Given  $\delta > 0$  and  $L \geq 0$ , there always exist  $a, b, p$  satisfying these conditions.

Figure 1 displays the lines  $x \mapsto 1$ ,  $x \mapsto 2(1-x)/\delta$  and  $x \mapsto (2x-1)/L$  for different values of the pair  $(\delta, L)$  with  $L > 0$ . The colored area corresponds to the points  $(a, b)$  satisfying the conditions (5.3) in the case  $p = 0$ , i.e. in the case where the numbers of Monte Carlo draws is constant over iterations. Note that this set becomes all the more restrictive that  $\delta \rightarrow 0$  and  $L \rightarrow \infty$ . Choosing  $p > 0$  gives more flexibility but it also leads to higher computational cost (since the number of Monte Carlo simulations increases along iterations).

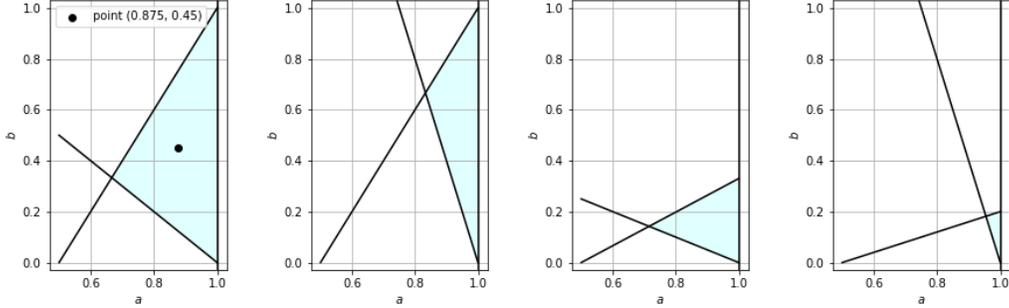


Figure 1: For different values of  $(\delta, L)$ , in the case  $p = 0$ , the colored area is the admissible set of points  $(a, b)$  satisfying (5.3). From left to right:  $(\delta, L) = (2, 1)$ ,  $(0.5, 1)$ ,  $(4, 3)$ , and  $(0.5, 5)$ .

## 5.2 Benchmark Problem

We consider the problem (3.1) in the case where

$$\Theta = [-\pi, \pi], \quad \pi(d\theta) = \frac{1}{2\pi} \mathbf{1}_{[-\pi, \pi]} d\theta, \quad (5.4)$$

the function  $H$  is given by

$$H(z, v, \theta) = (z - \phi^*(\theta)) \left( 1 + \frac{\cos(v)}{2} \sin(z - \phi^*(\theta)) \right) \quad (5.5)$$

with

$$\phi^*(\theta) = \left| \frac{4}{5} + \frac{1}{4} \exp(\sin(\theta)) - \cosh(\sin(\theta)^2) \right| (1 + \sin(2\theta)), \quad (5.6)$$

and, for any  $\theta \in \Theta$ , the conditional distribution  $\mu(\theta, dv)$  is a centered Gaussian law with variance  $\theta^2$ .

In real-life applications, the target function  $\phi^*$  is bound to be less challenging than the present one, e.g. monotone and/or convex/concave with respect to  $\theta$  or

some of its components (for instance in the context of financial applications, see e.g. [BCD<sup>+</sup>17]). Moreover, the user may be interested with a few coefficients  $u_i^*$  only, whereas we show numerical results up to  $m_K = 250$  below.

The choice of  $\mathcal{N}(0, \theta^2)$  for the kernel  $\mu(\theta, dv)$  is purely illustrative. This law could be replaced by any other one (simulatable i.i.d.) without expectable impact regarding the qualitative conclusions drawn from the numerical experiments below.

In this example,  $\mathbf{Is}(\mathcal{T}^*) = \{\phi^*\}$  and  $q = 1$ . The function  $h$  (cf. (1.1) and H3) is equal to

$$h(z, \theta) = (z - \phi^*(\theta)) \left( 1 + \frac{\mathbb{E}[\cos(\theta G)]}{2} \sin(z - \phi^*(\theta)) \right), \quad G \sim \mathcal{N}(0, 1). \quad (5.7)$$

It is easily checked that, for any  $z \in \mathbb{R}$  and  $\theta \in \Theta$ , we have

$$\begin{aligned} \int_{\mathcal{V}} |H(z, v, \theta)|^2 \mu(\theta, dv) &\leq 4|z - \phi^*(\theta)|^2, \\ (z - \phi^*(\theta)) \cdot h(z, \theta) &\geq \frac{1}{2}(z - \phi^*(\theta))^2. \end{aligned}$$

Hence, the assumptions H3, H4, H5, and H6 are satisfied.

Finally, for the orthonormal basis  $\{B_i, i \in \mathbb{N}\}$ , we choose the normalized trigonometric basis on  $\Theta = [-\pi, \pi]$  (cf. Example 1(v)). Therefore, we have  $\sup_{i \in \mathbb{N}} \sup_{\Theta} |B_i(\theta)| < +\infty$ , so that

$$Q_m = O(m),$$

i.e.  $L = 1$  in (5.1). Since  $\phi^*$  extended by periodicity outside  $[-\pi, \pi]$  is piecewise continuously differentiable, its truncation error satisfies (see Lemma 1)

$$\sum_{i=m+1}^{+\infty} |u_i^*|^2 = O(m^{-2}),$$

i.e. we have  $\delta = 2$  in (5.2). Numerically, one can check that the practical rate of convergence lies somewhere between 2 and 3, i.e. the theoretical value  $\delta = 2$  above is reasonably sharp (meaning that our example  $\phi^*$  is a “real”  $\delta = 2$  example and not “easier”).

### 5.3 Performance Criteria

In the numerical experiments that follow, we compare the performances of the algorithms with increasing  $m_k$  and fixed  $m$ , for different choices of  $(a, b, p)$ . The comparison relies on the root-mean-square errors, when the exact expectation

is approximated by the mean value over 50 independent runs of the algorithms. After  $K$  iterations, the square of the total error  $\mathcal{E}^2$  is decomposed into the mean squared SA error  $\mathcal{E}_{sa}^2$ , which is the error restricted to the  $(m_K + 1)$  estimated coefficients, and the squared truncation error  $\mathcal{E}_{tr}^2$ , i.e.  $\mathcal{E}^2 = \mathcal{E}_{sa}^2 + \mathcal{E}_{tr}^2$  where

$$\mathcal{E}^2 = \mathbb{E} \left[ \|u^K - u^*\|_{l_{2,q}}^2 \right], \quad \mathcal{E}_{sa}^2 = \mathbb{E} \left[ \sum_{i=0}^{m_K} (u_i^K - u_i^*)^2 \right], \quad \text{and} \quad \mathcal{E}_{tr}^2 = \sum_{i=m_K+1}^{+\infty} (u_i^*)^2$$

(recalling  $u_i^K = 0$  for  $i > m_K$ ). With the exception of Figure 4 that displays functions  $\phi^*$  and  $\phi^K$ , all our graphs are error plots in log-log scale.

## 5.4 Impact of the Increasing Dimension

In this section, we discuss the role of the sequence  $\{m_k, k \in \mathbb{N}\}$ . Since  $(\delta, L) = (2, 1)$ , the set of admissible pairs  $(a, b)$  for our example is given by the leftmost graph in Figure 1. When running the USA algorithm with increasing dimensions (i.e.  $b > 0$ ), we take  $(a, b) = (0.875, 0.45)$ , which lies in the middle of the admissibility set defined by (5.3) (not too close to the boundaries, see Figure 1, for ensuring a better numerical stability). The choice  $b = 0.45$  also follows from commonly used values for the number  $K$  of iterations in the algorithm and for the number  $m_K$  of the coefficients of interest: For instance, with  $b = 0.45$  and  $K = 10^4$ , we obtain  $m_K \approx K^b \approx 60$  coefficients (cf. (5.1)).

In Figure 2, we show that having  $m_k \rightarrow +\infty$  appears as a key feature from a numerical performance point of view, including for an accurate determination of the lower order coefficients (e.g. in the case where only the first few coefficients of the expansion of  $\phi^*$  are of interest to the user). In fact, as already mentioned in Section 2.3, the algorithm with fixed  $m$  does typically not converge to the first  $(m + 1)$  coefficients of the decomposition of  $\phi^*$ . In Figure 2[left], the  $L^2$ -error on the first 4 coefficients is displayed as a function of the number of iterations  $K$ , for two strategies on  $m_k$ : the solid line is the case  $m_k = O(k^b)$  with  $b = 0.45$  and the dotted line is the case  $m = 3$ . In Figure 2[right], the total error  $\mathcal{E}$  and the truncation error  $\mathcal{E}_{tr}$  are displayed, resp. in dash-dot line and dashed line in the case  $m_k$  is the constant sequence equal to  $m = 3$ . These figures show that, when  $m_k \rightarrow +\infty$ , USA converges (which is the claim of Theorem 1), whereas, when  $m_k = m$  for any  $k$ , it does not: the total error does not reach the truncation error since there is a non vanishing bias on the estimation of the first  $(m + 1)$  coefficients (the SA-error  $\mathcal{E}_{sa}$  does not vanish when  $K \rightarrow +\infty$ ).

Figure 3 displays the total error  $\mathcal{E}$  for different strategies on the sequence  $\{m_k, k \in \mathbb{N}\}$ : the solid line is the case  $m_k = \lfloor k^{0.45} \rfloor + 1$ , while the other lines correspond to the cases  $m_k = m = 10, 20, 30, 40$ , and 50. The algorithm with increasing  $m_k$  performs better throughout the whole path of USA. This holds

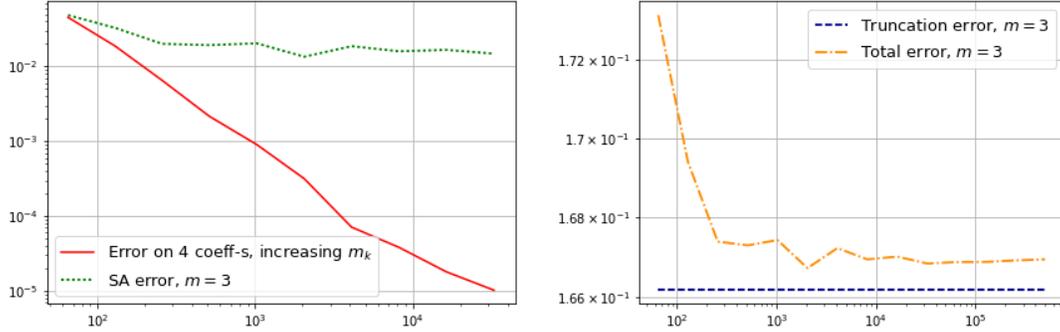


Figure 2: [left] In the case  $m_k \rightarrow \infty$  (solid line) and  $m_k = m = 3$  (dotted line), the error  $\mathbb{E} \left[ \sum_{i=0}^3 (u_i^K - u_i^*)^2 \right]^{1/2}$  as a function of the number of iterations  $K$ . [right] In the case  $m_k = m = 3$ , the truncation error  $\mathcal{E}_{tr}$  (dashed line) and the total error  $\mathcal{E}$  (dash-dot line) displayed as a function of  $K$ .

true in the burn-in phase, because, when  $m_k \rightarrow \infty$ , the dimension evolves with  $k$  (with larger values of  $\gamma_k$  naturally associated with the estimation of the first, larger coefficients), whereas, when  $m_k = m$  is constant, the dimension is too large in the beginning and the burn-in phase is longer. It is also true on the convergence part, where the fixed dimension algorithms  $m_k = m$  only converge up to a certain accuracy depending on the value of  $m$ .

Figure 4 displays the result of a single run of the USA algorithm. In dashed line, the function  $\theta \mapsto \phi^K(\theta)$  is displayed for  $\theta \in [-\pi, \pi]$ . For comparison, the function  $\theta \mapsto \phi^*(\theta)$  is displayed in solid line. We show the estimated function  $\phi^K$  for different values of  $K$  (from top to bottom,  $K \in \{128, 256, 512, 1024\}$ ) and for  $m_k$  increasing (left panels) versus  $m_k = m = 30$  for any  $k$  (right panels). The increasing dimension  $m_k$  leads to a smoother convergence, with intermediate iterations looking closer to a projection of  $\phi^*$  on the subspace spanned by a smaller number of basis functions.

## 5.5 Impact of the Design Parameters for the Increasing $m_k$ USA Algorithm

In this section, we discuss the choice of  $a, b, p$  when  $b > 0$  (see (5.1)).

### 5.5.1 Role of $b$

In this paragraph, we set  $a = 0.875, p = 0$ , and we compare different values of  $b \in \{0.3, 0.4, 0.5, 0.6, 0.7\}$ . The admissible values of  $b$  are in the range  $(0.125, 0.75)$ .

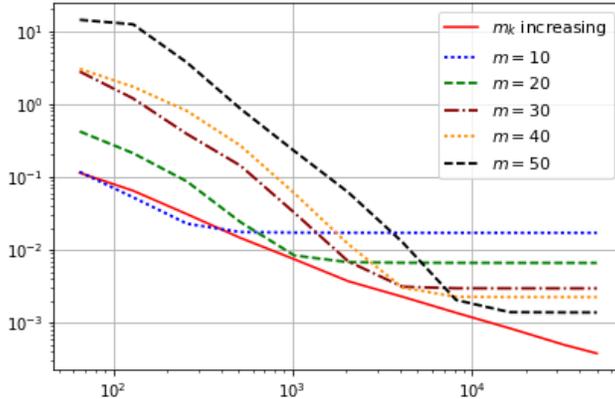


Figure 3: The total error  $\mathcal{E}$  as a function of the number of iterations, for different choices of the sequence  $\{m_k, k \in \mathbb{N}\}$ :  $m_k$  increasing (solid line) and  $m_k = m = 10, 20, 30, 40, 50$  (other lines).

Figure 5 displays the evolution of the total error  $\mathcal{E}$  as a function of the number of iterations  $K$  for different values of  $b$ . We observe that larger  $b$  leads to better convergence up to  $b = 0.70$ . However, as we may see, the gain in the speed of convergence from taking larger  $b$  decreases as we approach the border of the admissible interval. Moreover this analysis does not take into account higher computational cost due to a dimension growing faster when  $b$  is larger. For example, for  $b = 0.70$  we made only  $K = 2500$  iterations since the dimension becomes too large beyond this value. To conclude we suggest that optimal values of  $b$  (for given  $a$ ) in terms of both convergence and cost lie in the upper part of the admissible region but not too close to the boundary.

### 5.5.2 Role of $a$

In this paragraph, we set  $b = 0.45$ ,  $p = 0$ , and we compare different values of  $a \in \{0.75, 0.80, 0.85, 0.90, 0.95, 1\}$ : note that, since  $b = 0.45$ , the admissible values of  $a$  are in the range  $(0.725, 1.0]$  (see (5.3)).

Figure 6 displays the total error  $\mathcal{E}$  as a function of the number of iterations  $K$  for different values of  $a$ . We can see that the convergence for  $a = 1$  is not as good as for  $a < 1$ . To analyze this effect further, Figure 7 displays the SA-error (solid line) and the truncation error (dashed line) in the increasing  $m_k$  case, as well as the SA error (dash-dot line) for  $m_k = m = 10$ . The vertical line indicates the number of iterations when  $m_k$  reaches 10 in the increasing-dimension setting. The stepsize sequence  $\gamma_k = O(k^{-1})$  is well known to perform badly during the

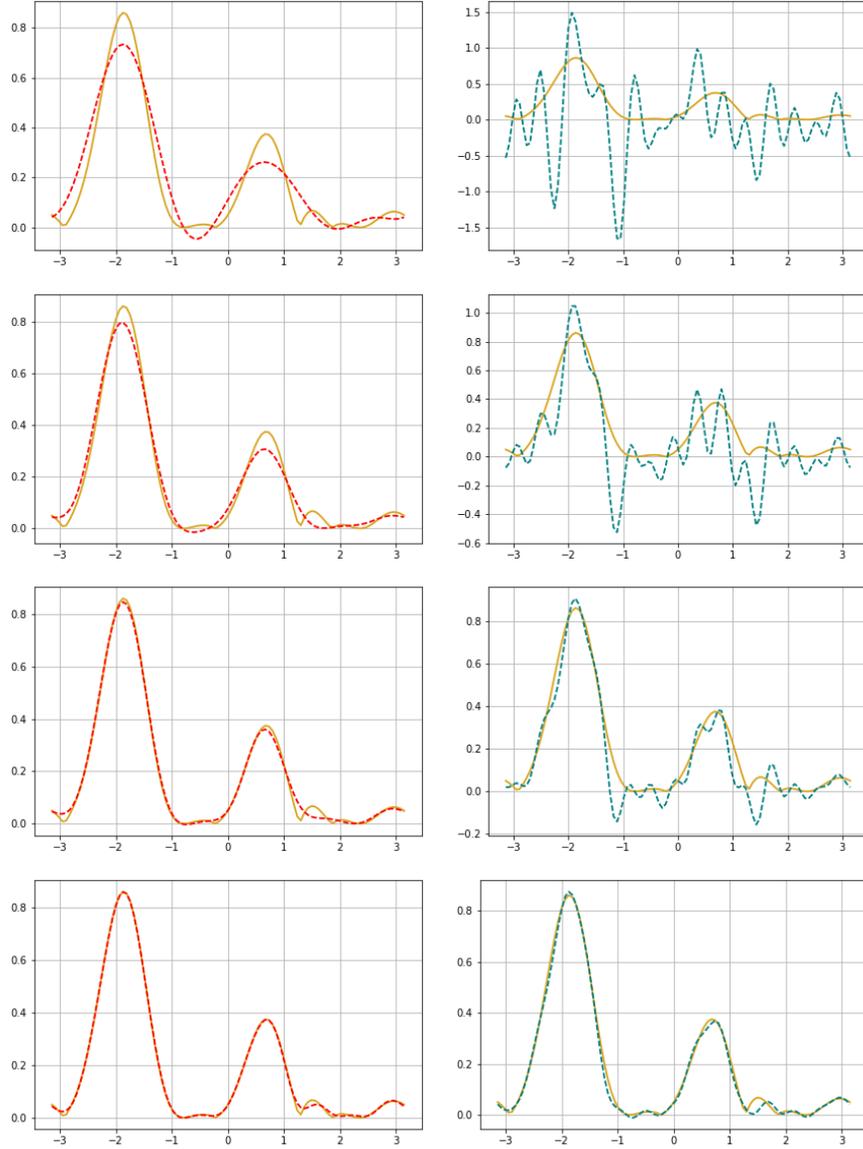


Figure 4: The functions  $\phi^*$  and  $\phi^K$  are displayed in respective solid line and dashed lines, as a function of  $\theta \in [-\pi, \pi]$ . On the left,  $\{m_k, k \in \mathbb{N}\}$  is increasing and on the right, it is constant and equal to  $m = 30$ . From top to bottom,  $K \in \{128, 256, 512, 1024\}$ .

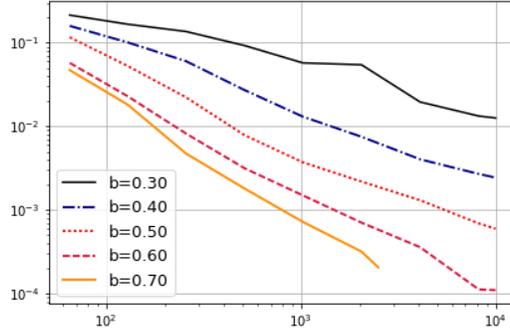


Figure 5: Total error  $\mathcal{E}$  as a function of the number of iterations  $K$ , for different values of  $b$  in  $\{0.3, 0.4, 0.5, 0.6, 0.7\}$ .

burn-in phase, since the steps are too small and do not allow to get quickly close to the solution. In our case, in the algorithm with increasing  $m_k$ , a coefficient  $u_i^*$  starts being estimated when the stepsize is  $\gamma_{k(i)}$  for  $k(i)$  such that  $m_{k(i)} = i$ . Hence, when  $\gamma_k$  decreases too fast, there are not enough iterations to estimate a given coefficient before a new one enters the scene; the algorithm does not have enough time to learn the successive coefficients and it produces a similar error on the first  $(m + 1)$  coefficients as the algorithm with fixed  $m_k = m$ . Thus, on Figure 7[left], the SA-error of the increasing  $m_k$ -algorithm is no better than the SA error of the fixed  $m_k = m$ -algorithm run for  $m = 10$ . On the contrary, for lower values of  $a$ , the total error is dominated by the truncation error of order  $m_k$  (see Figure 7[right] in the case  $a = 0.9$ ), which explains why such values of  $a$  yield to numerical convergence with similar (numerical) convergence rates.

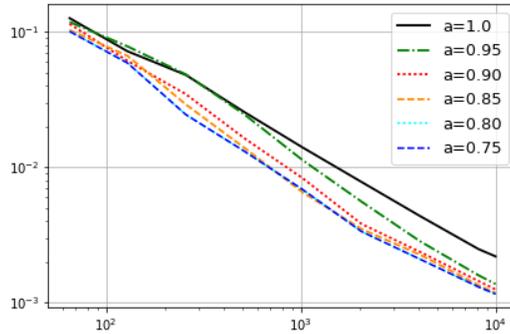


Figure 6: The total error  $\mathcal{E}$  as a function of the number of iterations, for different values of  $a$  in  $\{0.75, 0.80, 0.85, 0.9, 0.95, 1.0\}$ .

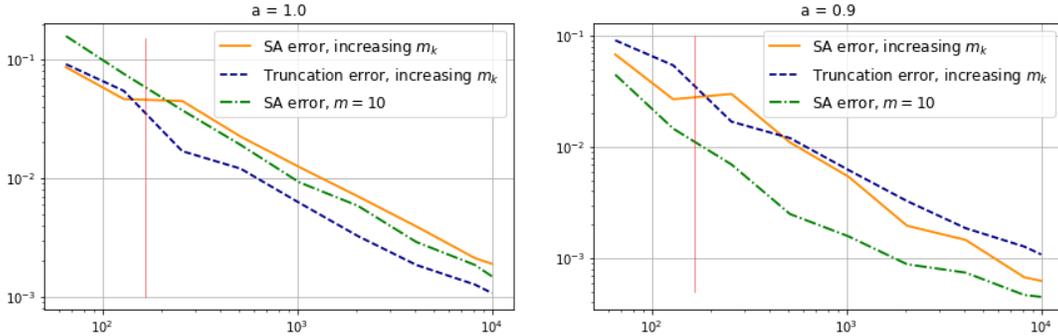


Figure 7: When  $a = 1$  [left] and  $a = 0.9$  [right], the SA-error  $\mathcal{E}_{sa}$  (solid line) and the truncation error  $\mathcal{E}_{tr}$  (dashed line) in the case  $m_k \rightarrow \infty$ . The SA-error  $\mathcal{E}_{sa}$  in the case  $m = 10$  is also displayed (dash-dot line). The vertical line shows the number of iterations  $k$  for which  $m_k$  reaches 10.

### 5.5.3 Role of $p$

In this section we consider the case  $p > 0$ , i.e. the number of Monte Carlo samples at each iteration increases along the USA iterations. One may check that all the triples of the parameters  $(a, b, p)$  used below lie in the admissible set (cf. (5.3)).

In the analyses below, we want to keep track of the dependence of the error with respect to a computational cost proxied by the total number of Monte Carlo draws of the pair  $(\theta, v)$ , i.e., after  $K$  iterations,  $\sum_{k=0}^{K-1} M_k \approx O(K^{p+1})$ . As we want to have the same dimension growth speed with respect to the computational cost for different tests, we take  $b = \bar{b}(p + 1)$  with  $\bar{b} = 0.45$ .

We first set  $a = 0.875$ . Figure 8 displays the total error  $\mathcal{E}$  as a function of the number of iterations (left) and as a function of the total number of Monte Carlo draws (right) for triples of the form  $(a, \bar{b}(p + 1), p)$  with various  $p$  and  $(a, \bar{b}) = (0.875, 0.45)$ . It shows that, even though larger  $p$  yield a better convergence in terms of the number of iterations  $K$ , there is no much difference when the computational cost is taken into account (i.e. in terms of the number of Monte Carlo draws).

Taking a larger  $p$  allows taking a smaller  $a$  (see (5.3)), so that  $\gamma_k$  decreases at a lower rate. To see if it is possible to take advantage of this balance, we test triples of the form  $(\bar{a}/(p + 1), \bar{b}(p + 1), p)$ , with  $(\bar{a}, \bar{b}) = (0.875, 0.45)$  and different values of  $p$ . Figure 9 displays the results. The conclusions are similar as for the previous test. Hence, on our problem, it seems difficult to take advantage of the degree of freedom provided by  $M_k$  by going beyond the obvious choice  $M_k = M$  for any  $k$ . Such a degree of freedom could still be useful to ensure the

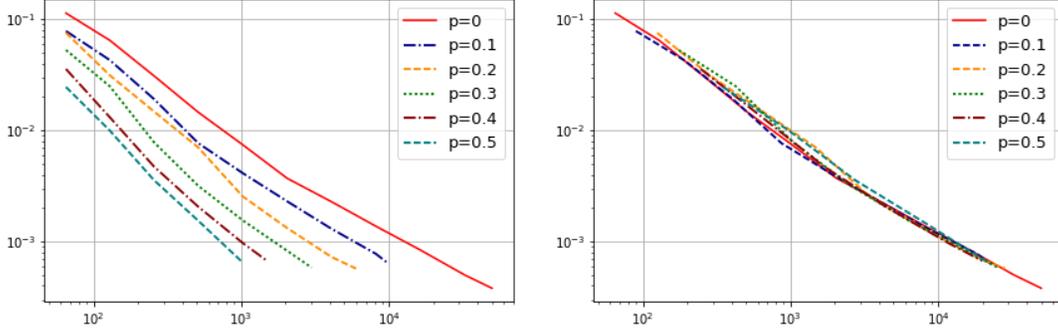


Figure 8: Total error  $\mathcal{E}$  of the USA algorithm for different values of  $p \in \{0, 0.1, 0.2, 0.3, 0.4, 0.5\}$  as a function of the number of iterations [left] and of the total number of Monte Carlo draws [right]. Here  $a = 0.875$  and  $b = 0.45(p + 1)$ .

convergence of  $\sum_{k \geq 0} \gamma_k^2 Q_{m_k} M_k^{-1}$  (as required by H2) in situations where  $L > 1$  (i.e.  $Q_m$  grows faster than in our example), and therefore ensure the convergence of the algorithm in such cases, even if this comes at a higher computational cost.

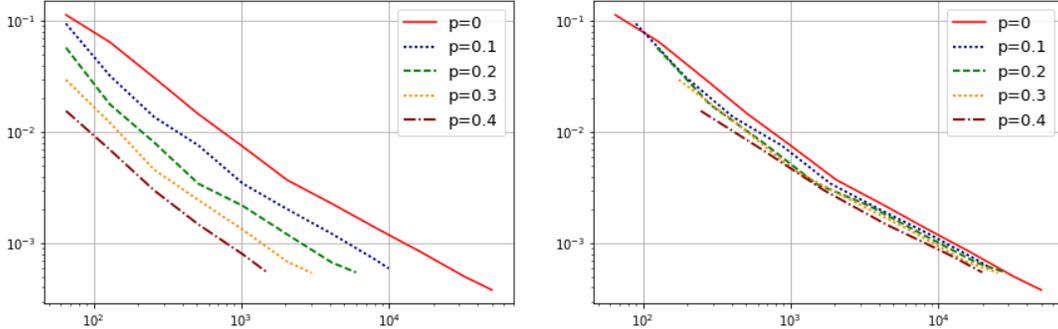


Figure 9: Total error  $\mathcal{E}$  of the USA algorithm for different values of  $p \in \{0, 0.1, 0.2, 0.3, 0.4\}$  as a function of the number of iterations [left] and of the total number of Monte Carlo draws [right]. Here  $a = 0.875/(p + 1)$  and  $b = 0.45(p + 1)$ .

In conclusion, we emphasize that the USA algorithm converges in all the studied cases for which the assumptions of Theorem 1 are verified. We can also observe in echo to Remark 3.4 that, in our numerics, the total error seems to converge at a rate of  $1/k^x$ , with  $x$  of varying from 0.5 to 1.0 depending, in particular, on the choice of the parameter  $b$ , with a higher  $b$  seeming to imply a faster convergence (but also more estimated coefficients and therefore a higher computational cost,

although the dependence of the latter on  $b$  is harder to analyze than the one on  $p$  studied in Section 5.5.3).

## A Truncation error for trigonometric basis

**Lemma 1.** *Let  $\phi : \mathbb{R} \rightarrow \mathbb{R}$  be  $2\pi$ -periodic and piecewise continuously differentiable. Let  $\{u_i, i \in \mathbb{N}\}$  be the coefficients of its decomposition with respect to the normalized trigonometric basis (cf. Example 1(v)). Then for some  $C > 0$*

$$\sum_{i=m+1}^{+\infty} |u_i|^2 \leq Cm^{-2}.$$

*Proof.* Let  $\phi^{2m+1}$  be the truncation of  $\phi$  using the first  $(2m+1)$  elements of the basis, i.e. the constant 1 and the normalized versions of the functions  $\cos(i\theta)$  and  $\sin(i\theta)$ ,  $i = 1, \dots, m$ . Let  $x \in [-\pi, \pi]$ . Define for  $t \in [-\pi, \pi]$

$$g(t) := \frac{\phi(x-t) - \phi(x)}{\sin(t/2)}.$$

By the computation stated in the proof of [Rud64, Theorem 8.14], we have

$$\phi^{2m+1}(x) - \phi(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(t) \cos(t/2) \sin(mt) dt + \frac{1}{2\pi} \int_{-\pi}^{\pi} g(t) \sin(t/2) \cos(mt) dt.$$

Using that  $\phi$  (and thus  $g$ ) is piecewise continuously differentiable we apply integration by parts and get

$$\begin{aligned} \phi^{2m+1}(x) - \phi(x) &= \frac{1}{2\pi m} \int_{-\pi}^{\pi} \frac{d}{dt} (g(t) \cos(t/2)) \cos(mt) dt \\ &\quad - \frac{1}{2\pi m} \int_{-\pi}^{\pi} \frac{d}{dt} (g(t) \sin(t/2)) \sin(mt) dt, \end{aligned}$$

which implies the result since  $\sum_{i>2m+1} |u_i|^2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} |\phi^{2m+1}(x) - \phi(x)|^2 dx$ .  $\square$

## B Compact sets in $l_{2,q}$

**Lemma 2.** *For a positive sequence  $\{a_n, n \in \mathbb{N}\}$  such that  $\sum_{i \geq 0} a_i^2 < \infty$  and an increasing sequence of non-negative integers  $\{d_n, n \in \mathbb{N}\}$  such that  $d_0 = 0$ , the closed convex set  $\mathcal{A}$ :*

$$\mathcal{A} := \left\{ u \in l_{2,q} : \sum_{d_n \leq i < d_{n+1}} |u_i|^2 \leq a_n^2 \quad \forall n \in \mathbb{N} \right\} \quad (\text{B.1})$$

*is compact.*

*Proof.* By [KB09, Theorem 3] a subset  $\mathcal{A}$  of  $l_{2,q}$  is relatively compact if and only if

$$\sup_{u \in \mathcal{A}} \sum_{i \geq n} |u_i|^2 \text{ is finite for every } n \text{ and converges to } 0 \text{ as } n \rightarrow +\infty.$$

For  $\mathcal{A}$  given by (B.1) it is clear that for  $l$  such that  $d_l \leq n$  we have

$$\sup_{u \in \mathcal{A}} \sum_{i \geq n} |u_i|^2 \leq \sup_{u \in \mathcal{A}} \sum_{i \geq d_l} |u_i|^2 \leq \sum_{j \geq l} a_j^2 \rightarrow 0$$

as  $n, l \rightarrow +\infty$ . Since  $\mathcal{A}$  is also closed we deduce that it is compact.  $\square$

**Corollary 2.** *Let  $\mathcal{A}$  be defined by (B.1) (with  $d_0$  not necessarily 0). For any constant  $B > 0$  the set  $\{u \in \mathcal{A} : \|u\|_{l_{2,q}} < B\}$  is convex compact.*

*Proof.* The result follows directly from Lemma 2 using that  $\sum_{i < d_0} |u_i|^2 \leq B^2$  for any  $u \in \mathcal{A}$ .  $\square$

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