Method of Partitioned Data Orthogonalisation for Principal Component Determination

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Abstract

In this paper, we propose and justify an estimator which allows us to estimate a random vector and its principal components from observed data with a higher associated accuracy and a better compression ratio than those by principal component analysis (PCA), for the same or smaller computational work as that by PCA. Such advantages are achieved under a certain condition which follows from a comparison of the error estimate associated with the presented method and that of PCA. The proposed estimator is implemented through a sequence of procedures which involve a partition of the observed data, a special orthogonalisation of the partitoned data, and the rank-constrained minimization of the associated error.
An extension of this technique to the case of the unconstrained error minimization is also studied. We give rigorous proofs of the statements associated with the proposed technique. The theory of the method is illustrated with results of numerical experiments using real data.

Keywords: Nonlinear filtering and estimation, pseudo-inverse operator, Karhunen-Loève transform.

1 Introduction

Principal component analysis (PCA) is the technique of multivariate analysis which determines the so-called 'principal components' of random data (Jolliffe 1986). The PCA is also known as the Karhunen-Loève transform in signal processing. To keep the uniform terminology, we use the same abbreviation, the PCA, for the Karhunen-Loève transform as well.

The PCA consists of two transforms. The first transform reduces the

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data to a 'shorter' random vector with the 'principal components' as its entries. The second transform restores the data from the 'shorter' random vector with a smallest possible error.

Application areas of PCA are abundant. They include, for example, feature selection and classification (Fukunaga 1999), clustering (Jolliffe 1986), forecasting (Stock and Watson 2002), noise suppression (Yamashita and Ogawa 1996), data compression (Scharf 1991a,b) etc. Due to such a variety of applications, and because of their increasing demand in the last decades, PCA has been extended in many directions.

According to Jolliffe (1986), PCA was originally proposed by Pearson (1901). Further developments of the PCA are due to Hotelling (1933), Karhunen (1947) and Loéve (1948). In the next section, we give a short overview of some recent relevant results.

1.1 Previous studies

The PCA can be reformulated as the best linear estimator of fixed rank (Torokhti and Howlett 2003b).

Let $\mathbf{x} \in L^2(\Omega, \mathbb{R}^m)$ and $\mathbf{y} \in L^2(\Omega, \mathbb{R}^n)$ be random vectors with realizations $\mathbf{x}(\omega) \in \mathbb{R}^m$ and $\mathbf{y}(\omega) \in \mathbb{R}^n$, respectively. Here, Ω is the set of outcomes of a probability space (Ω, Σ, μ), Σ is a σ–field of measurable subsets of Ω and $\mu : \Sigma \to [0, 1]$ is an associated probability measure on Σ with $\mu(\Omega) = 1$. Hereinafter, $\mathbf{y}$ is interpreted as observable data containing the vector $\mathbf{x}$ contaminated with noise. No relationship between $\mathbf{x}$ and noise is assumed to be known. We write $x = \mathbf{x}(\omega)$, $y = \mathbf{y}(\omega)$, etc so that $x = (x_1 \dots x_m)^T$ and $y = (y_1 \dots y_n)^T$.

Let $\mathbf{u} = (\mathbf{u}_1 \dots \mathbf{u}_m)^T \in L^2(\Omega, \mathbb{R}^m)$ and $\mathbf{v} = (\mathbf{v}_1 \dots \mathbf{v}_n)^T \in L^2(\Omega, \mathbb{R}^n)$ be any random vectors with $\mathbf{u}_i, \mathbf{v}_k \in L^2(\Omega, \mathbb{R})$ for $i = 1, \dots, m$, $k = 1, \dots, m$, and let $\|\mathbf{u}(\omega)\|$ be the 2-norm of $\mathbf{u}(\omega)$ (Golub and Van Loan 1996). We set

$$E[\|\mathbf{u}\|^2] = \int_\Omega \|\mathbf{u}(\omega)\|^2 d\mu(\omega) < \infty, \quad E[\mathbf{u}_i \mathbf{v}_k] = \int_\Omega \mathbf{u}_i(\omega)\mathbf{v}_k(\omega) d\mu(\omega) \quad (1)$$

and

$$E_{uv} = E[\mathbf{u}\mathbf{v}^T] = \{E[\mathbf{u}_i \mathbf{v}_k]\} \in \mathbb{R}^{m \times n} \quad (2)$$

for all $i = 1, \dots, m$, $k = 1, \dots, n$.

Let $\mathcal{P} : L^2(\Omega, \mathbb{R}^n) \to L^2(\Omega, \mathbb{R}^m)$ be a linear operator given by

$$[\mathcal{P}(\mathbf{y})](\omega) = P[\mathbf{y}(\omega)], \quad (3)$$

where $P \in \mathbb{R}^{m \times n}$, and let

$$J(\mathcal{P}) = E[||\mathbf{x} - \mathcal{P}(\mathbf{y})||^2]. \tag{4}$$

Consider the following problem. Find $\mathcal{P}^0 : L^2(\Omega, \mathbb{R}^n) \to L^2(\Omega, \mathbb{R}^m)$ such that

$$J(\mathcal{P}^0) = \min_{\mathcal{P}} J(\mathcal{P}) \tag{5}$$

subject to

$$\text{rank}(\mathcal{P}^0) = \eta \leq \min\{m, n\}. \tag{6}$$

Here, by definition (see, for example, Kowalski, Sikorski and Stenger, 1995),

$$\text{rank}(\mathcal{P}) = \dim \mathcal{P}(L^2(\Omega, \mathbb{R}^n)).$$

Similar to (3), we write $[\mathcal{P}^0(\mathbf{y})](\omega) = P^0[\mathbf{y}(\omega)]$ with $P^0 \in \mathbb{R}^{m \times n}$, and therefore the constraint in (6) can be represented in the form

$$\text{rank}(P^0) = \eta \leq \min\{m, n\}. \tag{7}$$

PCA solves this problem for the case when $\mathbf{y} = \mathbf{x}$, and the matrix E_{xx} is nonsingular. By the PCA, $\mathcal{P}^0$ is determined by the associated matrix P^0 constructed from the truncated eigendecomposition of E_{xx}.

Significant advances in the solution of the problem (5) have been achieved in recent decades. Tipping and Bishop (1999a,b) formulated PCA within a maximum-likehood framework. Roweis and Ghahramani (1999) represented PCA as a variation of unsupervised learning under a single basic generative model. Ocaña, Aguilera and Valderrama (1999), and Kneip and Utikal (2001) extended and applied PCA to functional data. Scharf (1991a,b) studied the problem (5) for the case when the covariance matrix $E[\mathbf{x}\mathbf{y}^T]$ is invertible. Yamashita and Ogawa (1996) studied PCA for the case when $\mathbf{x}$ is contaminated with an additive noise. Hua and Liu (1998) considered a version of the estimator (Scharf, 1991b) in terms of the pseudo-inverse for $E[\mathbf{x}\mathbf{y}^T]$. Stock and Watson (2002) used PCA for a forecasting problem. Honig and Xiao (2001) studied the performance of reduced-rank filtering based on PCA. Hua, Nikpour and Stoica (2001) advanced computational aspects of PCA. Relationships between the known reduced rank estimators are considered by Chen, Mitra and Schniter (2002).

We note that the estimators mentioned in the references above are linear. Yamada, Sekiguchi and Sakaniwa (2000), and Torokhti and Howlett (2001, 2002) developed nonlinear estimators.

1.2 Motivation

The previous studies motivate a further development of a random vector estimate in the following direction.

A performance of techniques based on PCA idea is characterized by the three parameters which are the compression ratio, the accuracy associated with the vector estimate and the required computational work. The compression ratio of PCA is

$$\kappa = \frac{\eta}{n}\,. \tag{8}$$

The computational work of the known PCA-like estimators is estimated by $\mathcal{O}(mn^2 + n^3)$ flops. In Section 2.3, we consider the related computational burden in more detail. The analytical representation of the associated error for PCA-like estimators is given in Section 2.3.

We wish to find an estimator which can improve the above characteristics. In other words, we wish to find an estimator which, under certain conditions, allows us to obtain a higher associated accuracy and a better compression ratio than those obtained by PCA, for the same or smaller computational work.

In the next sections, we establish conditions which imply such performance.

We call $\mathcal{P}$ in (3)–(5) the *homogeneous* estimator.

1.3 Basic idea

A device for the proposed method is as follows.

The observed data $\mathbf{y} \in L^2(\Omega, \mathbb{R}^n)$ are partitioned in 'shorter' vectors $\mathbf{z}_1, \ldots, \mathbf{z}_s$ such that $\mathbf{z}_i \in L^2(\Omega, \mathbb{R}^{n_i})$ for $i = 1, \ldots, s$ where $n_1 + \cdots + n_s = n$. Then $\mathbf{z}_1, \ldots, \mathbf{z}_s$ are transformed to orthogonal vectors $\mathbf{v}_1, \ldots, \mathbf{v}_s$ (see Definition 1 and Lemma 2 ahead.) A desired estimator follows from the solution of the constrained minimization problem given by (17)–(22), formulated in Section 2.1, which is posed in terms of vectors $\mathbf{v}_1, \ldots, \mathbf{v}_s$.

We note that our estimator $\hat{\mathcal{P}}$, presented by (18) below, is non-linear due to the term q and we call $\hat{\mathcal{P}}$ the *non-homogeneous* estimator.

Unlike the problem (5), which is formulated for one constraint only, the problem (17)–(22) is subject to s constraints (21) with $s = 1, 2, \ldots$. As a result, the estimator $\hat{\mathcal{P}}$ is determined by s matrices of small sizes $m \times n_i$ and $n_i \times n_i$ (see Lemma 3) while PCA-like techniques imply computation of larger $m \times n$ and $n \times n$ matrices.

Such a special form of the estimator $\hat{\mathcal{P}}$ implies advantages related to the associated accuracy, compression ratio and computational work. In particular, evaluations involving $m \times n_i$ and $n_i \times n_i$ matrices require less computational work than that for larger $m \times n$ and $n \times n$ matrices. A more detailed discussion in this regard is given in Section 2.3. Differences from some other known techniques are discussed in Sections 2.1 and 2.2.

We show that, similar to PCA, our estimator can be represented as a composition of two transforms. The first of them is to determine the principal components, and the second transform is to restore the reference vector.

The method which implies such a *non-homogeneous* estimator will be called the method of partitioned data orthogonalisation.

2 Method of partitioned data orthogonalisation

A formalisation of the device described above is as follows.

Let $\mathcal{Z} : L^2(\Omega, \mathbb{R}^n) \to L^2(\Omega, \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_s})$ and $\mathcal{Z}_i : L^2(\Omega, \mathbb{R}^n) \to L^2(\Omega, \mathbb{R}^{n_i})$ be such that

$$\mathcal{Z}(\mathbf{y}) = (\mathcal{Z}_1(\mathbf{y}) \ldots \mathcal{Z}_s(\mathbf{y})), \quad \mathcal{Z}_i(\mathbf{y}) = \mathbf{z}_i \quad \text{and} \quad [\mathcal{Z}(\mathbf{y})](\omega) = (z_1^T \ldots z_s^T)^T, \tag{9}$$

where $\mathbf{z}_i \in L^2(\Omega, \mathbb{R}^{n_i})$, $z_i = \mathbf{z}_i(\omega)$, $i = 1, \ldots, s$ and $n_1 + \cdots + n_s = n$. We call $\mathcal{Z}$ the partitioning operator.

Next, let $P \in \mathbb{R}^{m \times n}$ be a matrix composed from a matrix $A \in \mathbb{R}^{m \times n}$ and a block diagonal matrix $B \in \mathbb{R}^{n \times n}$ so that

$$P = AB = [A_1 \ldots A_s] \begin{bmatrix} B_1 & \mathbb{O} & \ldots & \mathbb{O} \\ \mathbb{O} & B_2 & \ldots & \mathbb{O} \\ \ldots & \ldots & \ldots & \ldots \\ \mathbb{O} & \ldots & \mathbb{O} & B_s \end{bmatrix}, \tag{10}$$

where $\mathbb{O}$ is the zero matrix, $A_i \in \mathbb{R}^{m \times n_i}$ and $B_i \in \mathbb{R}^{n_i \times n_i}$.

Then

$$Py = [A_1 \ldots A_s] \begin{bmatrix} B_1 & \mathbb{O} & \ldots & \mathbb{O} \\ \mathbb{O} & B_2 & \ldots & \mathbb{O} \\ \ldots & \ldots & \ldots & \ldots \\ \mathbb{O} & \ldots & \mathbb{O} & B_s \end{bmatrix} \begin{bmatrix} z_1 \\ \ldots \\ z_s \end{bmatrix} = \sum_{i=1}^{s} A_i B_i z_i, \tag{11}$$

where $z_i = \mathbf{z}_i(\omega)$ for all $i = 1, \ldots, s$.

Let

$$\mathcal{A} : L^2(\Omega, \mathbb{R}^n) \to L^2(\Omega, \mathbb{R}^m), \quad \mathcal{A}_i : L^2(\Omega, \mathbb{R}^{n_i}) \to L^2(\Omega, \mathbb{R}^m), \tag{12}$$

$$\mathcal{B} : L^2(\Omega, \mathbb{R}^n) \to L^2(\Omega, \mathbb{R}^n) \quad \text{and} \quad \mathcal{B}_i : L^2(\Omega, \mathbb{R}^{n_i}) \to L^2(\Omega, \mathbb{R}^{n_i}) \tag{13}$$

be continuous operators associated with the matrices above by the equations

$$[\mathcal{B}_i(\mathbf{z}_i)](\omega) = B_i[\mathbf{z}_i(\omega)], \quad [\mathcal{A}_i(\mathbf{b}_i)](\omega) = A_i[\mathbf{b}_i(\omega)], \tag{14}$$

$$[\mathcal{B}(\mathbf{y})](\omega) = B[\mathbf{y}(\omega)], \quad \text{and} \quad [\mathcal{A}(\mathbf{b})](\omega) = A[\mathbf{b}(\omega)], \tag{15}$$

where, for $i = 1, \ldots, s$,

$$\mathbf{b}_i = \mathcal{B}_i(\mathbf{z}_i) \quad \text{and} \quad \mathbf{b} = \mathcal{B}(\mathbf{y}).$$

The operators $\mathcal{A}_i$, $\mathcal{B}_i$ will be determined from the problem formulated in the next section. An operator $\hat{\mathcal{P}}$ composed from operators $\mathcal{A}_i$, $\mathcal{B}_i$ with $i = 1, \ldots, s$ represents the estimator which we wish to construct.

Before the statement of the problem, we formulate a definition of orthogonality.

For any random vectors $\mathbf{u} \in L^2(\Omega, \mathbb{R}^m)$ and $\mathbf{v} \in L^2(\Omega, \mathbb{R}^n)$, we write

$$\mathbb{E}_{uv} = E_{uv} - E[\mathbf{u}]E[\mathbf{v}^T]. \tag{16}$$

Definition 1 *The set of random vectors* $\mathbf{b}_1, \ldots, \mathbf{b}_s \in L^2(\Omega, \mathbb{R}^{n_i})$ *is called pairwise orthogonal if*

$$\mathbb{E}_{b_i b_j} = \mathbb{O}$$

for any $i \neq j$ *with* $i, j = 1, \ldots, s$.

Definition 2 *The operators* $\mathcal{B}_1, \ldots, \mathcal{B}_s$ *are called orthogonal if vectors* $\mathbf{b}_1, \ldots, \mathbf{b}_s$ *are pairwise orthogonal.*

2.1 Statement of the problem

Let

$$J(q, \mathcal{A}_1, \ldots, \mathcal{A}_s) = E[\|\mathbf{x} - (q + \sum_{i=1}^{s} \mathcal{A}_i \mathcal{B}_i \mathcal{Z}_i(\mathbf{y}))\|^2]. \tag{17}$$

The problem is to find a *non-homogeneous* estimator $\hat{\mathcal{P}}$,

$$\begin{aligned} \hat{\mathcal{P}}(\mathbf{y}) &= \hat{q} + \hat{\mathcal{A}}_i \hat{\mathcal{B}}_i \mathcal{Z}_i(\mathbf{y}) + \ldots + \hat{\mathcal{A}}_i \hat{\mathcal{B}}_i \mathcal{Z}_i(\mathbf{y}) \\ &= \hat{q} + \sum_{i=1}^{s} \hat{\mathcal{A}}_i \hat{\mathcal{B}}_i \mathcal{Z}_i(\mathbf{y}), \end{aligned} \tag{18}$$

with q, $\hat{\mathcal{A}}_1$, ..., $\hat{\mathcal{A}}_s$ and $\hat{\mathcal{B}}_1$, ..., $\hat{\mathcal{B}}_s$ such that

$$\begin{aligned} &\text{(i)} \quad \hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s \quad \text{are orthogonal operators, and} \\ &\text{(ii)} \quad \hat{q}, \hat{\mathcal{A}}_1, \ldots, \hat{\mathcal{A}}_s \quad \text{satisfy the condition} \end{aligned} \tag{19}$$

$$J(\hat{q}, \hat{\mathcal{A}}_1, \ldots, \hat{\mathcal{A}}_s) = \min_{\mathbf{q}, \mathcal{A}_1, \ldots, \mathcal{A}_s} J(q, \mathcal{A}_1, \ldots, \mathcal{A}_s) \tag{20}$$

subject to

$$\begin{aligned} &\text{rank}\,(\hat{\mathcal{A}}_1) = \eta_1, \quad \ldots, \quad \text{rank}\,(\hat{\mathcal{A}}_s) = \eta_s \\ &\text{with} \quad \eta_i \leq \min\{m, n_i\} \quad \text{for each} \quad i = 1, \ldots, s. \end{aligned} \tag{21}$$

In matrix notation, the constraints (21) mean that

$$\text{rank}\,(\hat{A}_1) = \eta_1, \quad \ldots, \quad \text{rank}\,(\hat{A}_s) = \eta_s. \tag{22}$$

Hence, the estimator $\hat{\mathcal{P}}$ is defined by the partitioning operator $\mathcal{Z}$, the orthogonalisation operators $\hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s$, the minimizing operators $\hat{\mathcal{A}}_1, \ldots, \hat{\mathcal{A}}_s$, and the term $\hat{q}$.

Remark 1 *The distinctive step in the problem under consideration is the partitioning of the data* $\mathbf{y}$ *whilst retaining the vector* $\mathbf{x}$ *in its unpartitioned form. Of course, one can treat* $\mathbf{x}$ *as* $\mathbf{x} = (\boldsymbol{\kappa}_1, ..., \boldsymbol{\kappa}_s)$ *with* $\boldsymbol{\kappa}_i \in L^2(\Omega, \mathbb{R}^{m_i})$ *and* $m_1 + \ldots + m_s = m$*, and then consider an estimate of each part of* $\mathbf{x}$*,* $\boldsymbol{\kappa}_i$*, from a corresponding part of data* $\mathbf{y}$*,* $\mathbf{z}_i$*, and applying PCA to each pair* $\boldsymbol{\kappa}_i, \mathbf{z}_i$*. We call such a process the partitioned PCA. This procedure is not a device of the proposed method because in such a case, we come to the problem that differs from* (5) *by notation only. In our approach, we estimate the entire vector* $\mathbf{x}$ *from data* $\mathbf{y}$ *transformed in a special way. In Section 3.2, we give a comparative numerical analysis for partitioned PCA and our estimator.*

Remark 2 *There are specific differences between the proposed approach and the known techniques developed, in particular, by Yamada, Sekiguchi and Sakaniwa* (2000)*, Hua, Nikpour and Stoica* (2001) *and Torokhti and Howlett* (2001, 2002, 2003*a*, *b*)*. The methods by Yamada, Sekiguchi and Sakaniwa* (2000)*, and Torokhti and Howlett* (2001, 2002) *are based on polynomial operators. The proposed estimator is not polynomial. Hua, Nikpour and Stoica* (2001) *considered an advanced power method for computing the matrix which implements PCA. Although the proposed method is not PCA, the technique by Hua, Nikpour and Stoica* (2001) *can be applied here as*

well. The methods by Torokhti and Howlett (2003*a*, *b*) *are based on specific iterative procedures. Unlike the techniques (Torokhti and Howlett* 2003*a*, *b*), *the proposed estimator relates to so called direct estimators, which are not iterative. We would also like to mention that techniques of establishing the main results given in Lemmas* 2 *and* 3 *below are different from the techniques used by Torokhti and Howlett* (2001, 2002, 2003*a*, *b*). *In particular,* $\mathcal{A}_1$, ..., $\mathcal{A}_s$ *are operators, not matrices, and this circumstance implies new specific derivations given in the proof of Lemma* 3.

2.2 Solution of the problem

2.2.1 Determination of $\hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s$

First, we determine $\hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s$. The following preparatory result is used in the subsequent derivation. Hereinafter, the symbol † is used to denote the pseudo-inverse operator (Ben-Israel and Greville 1974).

Lemma 1 (Torokhti and Howlett 2001) *For any random vectors* $\mathbf{g} \in L^2(\Omega, \mathbb{R}^m)$ *and* $\mathbf{h} \in L^2(\Omega, \mathbb{R}^n)$,

$$\mathbb{E}_{gh}\mathbb{E}_{hh}^{\dagger}\mathbb{E}_{hh} = \mathbb{E}_{gh}. \tag{23}$$

□

Now, we are in a position to find $\hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s$.

Lemma 2 *Let* $\mathbf{b}_i = \mathcal{B}_i(\mathbf{z}_i)$ *and let* $\mathcal{G}_{ik} : L^2(\Omega, \mathbb{R}^n) \to L^2(\Omega, \mathbb{R}^n)$ *be defined by*

$$[\mathcal{G}_{ik}(\mathbf{b}_k)](\omega) = G_{ik}[\mathbf{b}_k(\omega)],$$

where

$$G_{ik} = E_{z_i b_k} E_{b_k b_k}^{\dagger} + M_{ik}(I - E_{b_k b_k} E_{b_k b_k}^{\dagger}) \tag{24}$$

with $M_{ik} \in \mathbb{R}^{n_i \times n_i}$ *arbitrary and* I *the identity matrix. Then the operators* $\hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s$, *defined by*

$$\hat{\mathcal{B}}_1(\mathbf{z}_1) = \mathbf{z}_1 \quad \textit{and} \quad \hat{\mathcal{B}}_i(\mathbf{z}_i) = \mathbf{z}_i - \sum_{k=1}^{i-1} \mathcal{G}_{ik}(\mathbf{b}_k) \quad \textit{for} \quad i = 2, \ldots, p, \tag{25}$$

are orthogonal.

Proof : We wish that $\mathbb{E}_{b_i b_k} = \mathbb{O}$ for $i \neq k$. If G_{ik} has been chosen so that this condition is true for all $k = 1, \ldots, i-1$ then we have

$$E[(\mathbf{z}_i - \sum_{l=1}^{i-1} \mathcal{G}_{il}(\mathbf{b}_l)\mathbf{b}_k^T] = E_{z_i b_k} - \sum_{l=1}^{i-1} G_{il} E_{b_l b_k} = E_{z_i b_k} - G_{ik} E_{b_k b_k} = \mathbb{O}. \quad (26)$$

Thus,

$$G_{il} E_{b_k b_k} = E_{z_i b_k}. \quad (27)$$

The neccessary and sufficient condition (Ben-Israel and Greville 1974) for the solution of the matrix equation (27) is given by

$$E_{z_i b_k} E_{b_k b_k}^{\dagger} E_{b_k b_k} = E_{z_i b_k}. \quad (28)$$

By Lemma 1, (28) is true. Then the general solution to (27) (by Ben-Israel and Greville 1974) is given by (24). □

Remark 3 *the idea of random vector orthogonalisation is not, of course, new. In particular, Goldstein, Reed and Scharf* (1998)*, and Mathews and Sicuranza* (2001) *have considered generalisations of the Gram-Schmidt orthogonalisation procedure, but for problems which are different from the one studied here. In the context of the proposed approach, the novelty of the procedure* (24), (25) *is a generalisation of the Gram-Schmidt technique to the case when* $\mathcal{B}_1$, ..., $\mathcal{B}_s$ *are operators, not matrices as in the known references, and when* $\mathcal{B}_1$, ..., $\mathcal{B}_s$ *are not invertible. Therefore Lemma 2 establishes the orthogonalisation process in terms of the pseudo-inverse operator. Additionally, the orthogonalisation by* (24), (25) *is aimed at a new implementation into the structure of the estimator* $\hat{\mathcal{P}}$ *by Lemma 3 below. It is also worthwhile to note that Lemma 2 establishes nonuniqueness of the orthogonal operators* $\hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s$ *due to arbitrary matrices* M_{ik} *in* (24)*.*

2.2.2 Determination of $\hat{q}$ and $\hat{\mathcal{A}}_1$, ..., $\hat{\mathcal{A}}_s$

The vector $\hat{q}$ and operators $\hat{\mathcal{A}}_1$, ..., $\hat{\mathcal{A}}_s$ satisfying (20)–(21) are defined by the following procedure. For each $i = 1, \ldots, s$, let $U_i D_i V_i^T$ be the singular value decomposition (SVD) of $\mathbb{E}_{x b_i} (\mathbb{E}_{b_i b_i}^{1/2})^{\dagger}$,

$$U_i D_i V_i^T = \mathbb{E}_{x b_i} (\mathbb{E}_{b_i b_i}^{1/2})^{\dagger}, \quad (29)$$

where $U_i \in \mathbb{R}^{m \times n_i}$, $V_i \in \mathbb{R}^{n_i \times n_i}$ are orthogonal and $D_i \in \mathbb{R}^{n_i \times n_i}$ is diagonal,

$$U_i = [s_{i1}, \ldots, s_{in_i}], \quad V_i = [q_{i1}, \ldots, q_{in_i}] \quad \text{and} \quad D_i = \mathrm{diag}(\sigma_{i1}, \ldots, \sigma_{in_i}), \quad (30)$$

with $\sigma_{i1} \geq \cdots \geq \sigma_{ip_i} > 0$ and $\sigma_{i,p_i+1} = \cdots = \sigma_{in_i} = 0$.

We set

$$U_{\eta_i} = [s_{i1}, \ldots, s_{i\eta_i}], \quad V_{\eta_i} = [q_{i1}, \ldots, q_{i\eta_i}] \quad \text{and} \quad D_{\eta_i} = \text{diag}(\sigma_{i1}, \ldots, \sigma_{i\eta_i}),$$

where $U_{\eta_i} \in \mathbb{R}^{m \times \eta_i}$, $V_{\eta_i} \in \mathbb{R}^{\eta_i \times \eta_i}$ and $D_{\eta_i} \in \mathbb{R}^{\eta_i \times \eta_i}$. Now we define $T_{\eta_i} \in \mathbb{R}^{m \times n_i}$ and $\mathcal{T}_{\eta_i} : L^2(\Omega, \mathbb{R}^{n_i}) \to L^2(\Omega, \mathbb{R}^m)$ by

$$T_{\eta_i} = U_{\eta_i} D_{\eta_i} V_{\eta_i}^T \quad \text{and} \quad [\mathcal{T}_{\eta_i}(\mathbf{g}_i)](\omega) = T_{\eta_i}[\mathbf{g}_i(\omega)], \tag{31}$$

respectively, for any $\mathbf{g}_i : L^2(\Omega, \mathbb{R}^{n_i})$.

We also define operators $\mathcal{E}_{b_i b_i} : L^2(\Omega, \mathbb{R}^{n_i}) \to L^2(\Omega, \mathbb{R}^{n_i})$ and $\mathcal{M}_i : L^2(\Omega, \mathbb{R}^{n_i}) \to L^2(\Omega, \mathbb{R}^m)$ by the equations

$$[\mathcal{E}_{b_i b_i}(\mathbf{b}_i)](\omega) = \mathbb{E}_{b_i b_i}[\mathbf{b}_i(\omega)] \quad \text{and} \quad [\mathcal{M}_i(\mathbf{b}_i)](\omega) = M_i[\mathbf{b}_i(\omega)], \tag{32}$$

with arbitrary $M_i \in \mathbb{R}^{m \times n_i}$ for every $i = 1, \ldots, s$. Operators $\mathcal{E}^\dagger_{b_i b_i}$ and $(\mathcal{E}^{1/2}_{b_i b_i})^\dagger$ are defined by matrices $\mathbb{E}^\dagger_{b_i b_i}$ and $(\mathbb{E}^{1/2}_{b_i b_i})^\dagger$ with equations similar to that defining $\mathcal{E}_{b_i b_i}$.

The symbol $\mathcal{I}$ denotes the identity operator.

Lemma 3 *The vector $\hat{q}$ and operators $\hat{\mathcal{A}}_1$, ..., $\hat{\mathcal{A}}_s$, satisfying* (20) *and* (21)*, are determined by*

$$\hat{q} = E[\mathbf{x}] - \sum_{i=1}^{s} \hat{A}_i E[\mathbf{b}_i] \tag{33}$$

and

$$\begin{aligned} \hat{\mathcal{A}}_1 &= \mathcal{T}_{\eta_1}(\mathcal{E}^{1/2}_{b_1 b_1})^\dagger + \mathcal{M}_1(\mathcal{I} - \mathcal{E}_{b_1 b_1}\mathcal{E}^\dagger_{b_1 b_1}), && (34) \\ &\vdots \\ \hat{\mathcal{A}}_s &= \mathcal{T}_{\eta_s}(\mathcal{E}^{1/2}_{b_s b_s})^\dagger + \mathcal{M}_s(\mathcal{I} - \mathcal{E}_{b_s b_s}\mathcal{E}^\dagger_{b_s b_s}). && (35) \end{aligned}$$

Proof: For any random vector $\mathbf{h}$, $E[\|\mathbf{h}\|^2] = \text{tr}\{E[\mathbf{h}\mathbf{h}^T]\}$. We have

$$\begin{aligned} J(q, \mathcal{A}_1, \ldots, \mathcal{A}_s) &= \text{tr}[E_{xx} - E[\mathbf{x}]q^T - \sum_{i=1}^{s} E_{xb_i} A_i^T - qE[\mathbf{x}^T] \\ &+ qq^T + q\sum_{i=1}^{s} E[\mathbf{b}_i^T] A_i^T - \sum_{i=1}^{s} A_i E_{b_i x} \qquad (36) \\ &+ \sum_{i=1}^{s} A_i E[\mathbf{b}_i] q^T + E(\sum_{i=1}^{s} A_i \mathbf{b}_i \sum_{k=1}^{s} \mathbf{b}_k^T A_k^T)]. \end{aligned}$$

At the same time, $J(q, \mathcal{A}_1, \ldots, \mathcal{A}_s)$ can be represented as

$$J(q, \mathcal{A}_1, \ldots, \mathcal{A}_s) = J_0 + J_1 + J_2, \tag{37}$$

where

$$J_0 = ||\mathbb{E}_{xx}^{1/2}||^2 - \sum_{i=1}^{s} ||\mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}||^2, \tag{38}$$

$$J_1 = ||q - E[\mathbf{x}] + \sum_{i=1}^{s} A_i E[\mathbf{b}_i]||^2 \quad \text{and} \quad J_2 = \sum_{i=1}^{s} ||A_i\mathbb{E}_{b_ib_i}^{1/2} - \mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}||^2 \tag{39}$$

To show that (37) is true, we use the relationships

$$\mathbb{E}_{xb_i}\mathbb{E}_{b_ib_i}^{\dagger}\mathbb{E}_{b_ib_i} = \mathbb{E}_{xb_i} \quad \text{and} \quad \mathbb{E}_{b_ib_i}^{\dagger}\mathbb{E}_{b_ib_i}^{1/2} = (\mathbb{E}_{b_ib_i}^{\dagger})^{1/2},$$

(see Torokhti and Howlett 2001). Then

$$\begin{aligned} J_1 &= \operatorname{tr}(qq^T - qE[\mathbf{x}^T] + \sum_{i=1}^{s} qE[\mathbf{b}_i^T]A_i + E[\mathbf{x}]E[\mathbf{x}^T] \\ &- E[\mathbf{x}]q^T - \sum_{i=1}^{s} E[\mathbf{x}]E[\mathbf{b}_i^T]A_i^T + \sum_{i=1}^{s} A_iE[\mathbf{b}_i]q^T \\ &- \sum_{i=1}^{s} A_iE[\mathbf{b}_i]E[\mathbf{x}^T] + \sum_{i=1}^{s} A_iE[\mathbf{b}_i]\sum_{k=1}^{s} E[\mathbf{b}_i^T]A_i^T) \end{aligned} \tag{40}$$

and

$$\begin{aligned} J_2 &= \sum_{i=1}^{s} \operatorname{tr}(A_i - \mathbb{E}_{xb_i}\mathbb{E}_{b_ib_i}^{\dagger})\mathbb{E}_{b_ib_i}(A_i^T - \mathbb{E}_{b_ib_i}^{\dagger}\mathbb{E}_{b_ix}) \\ &= \sum_{i=1}^{s} \operatorname{tr}(A_i\mathbb{E}_{b_ib_i}A_i^T - A_i\mathbb{E}_{b_ix} - \mathbb{E}_{xb_i}A_i^T + \mathbb{E}_{xb_i}\mathbb{E}_{b_ib_i}^{\dagger}\mathbb{E}_{b_ix}), \end{aligned} \tag{41}$$

where

$$\begin{aligned} \sum_{i=1}^{s} \operatorname{tr}(A_i\mathbb{E}_{b_ib_i}A_1^T) &= \operatorname{tr}[E(\sum_{i=1}^{s} A_i\mathbf{b}_i \sum_{k=1}^{s} \mathbf{b}_k^T A_k^T)] \\ &- \operatorname{tr}(\sum_{i=1}^{s} A_iE[\mathbf{b}_i]\sum_{k=1}^{s} E[\mathbf{b}_i^T]A_i^T) \end{aligned} \tag{42}$$

because

$$E[\mathbf{b}_i\mathbf{b}_k^T] - E[\mathbf{b}_i]E[\mathbf{b}_k^T] = \mathbb{O} \quad \text{for} \quad i \neq k$$

due to orthogonality of vectors $\mathbf{b}_1, \ldots, \mathbf{b}_s$.

It follows from (36)–(42) that (36) and (37) are equivalent. Hence,

$$\begin{aligned} J(q, \mathcal{A}_1, \ldots, \mathcal{A}_s) &= \|\mathbb{E}_{xx}^{1/2}\|^2 - \sum_{i=1}^{s} \|\mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}\|^2 + \|q - E[\mathbf{x}] + \sum_{i=1}^{s} A_i E[\mathbf{b}_i]\|^2 \\ &+ \sum_{i=1}^{s} \|A_i\mathbb{E}_{b_ib_i}^{1/2} - \mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}\|^2. \end{aligned} \tag{43}$$

The constrained minimum (20)–(22) is achieved if $q = \hat{q}$ by (33), and

$$A_i\mathbb{E}_{b_ib_i}^{1/2} = T_{\eta_i}. \tag{44}$$

The matrix equation (44) has the general solution (Ben-Israel and Greville 1974)

$$A_i = T_{\eta_i}(\mathbb{E}_{b_ib_i}^{1/2})^{\dagger} + M_i[I - \mathbb{E}_{b_ib_i}^{1/2}(\mathbb{E}_{b_ib_i}^{1/2})^{\dagger}] \tag{45}$$

if and only if

$$T_{\eta_i}(\mathbb{E}_{b_ib_i}^{1/2})^{\dagger}\mathbb{E}_{b_ib_i}^{1/2} = T_{\eta_i}. \tag{46}$$

The latter is satisfied on the basis of the following derivation.

As an extension of the technique presented in the proof of Lemmas 1 and 2 by Torokhti and Howlett (2001), it can be shown that for any matrices $Q_1, Q_2 \in \mathbb{R}^{m\times n}$,

$$\mathcal{N}(Q_1) \subseteq \mathcal{N}(Q_2) \tag{47}$$

implies

$$Q_2(I - Q_1^{\dagger}Q_1) = \mathbb{O}, \tag{48}$$

where $\mathcal{N}(Q_i)$ is the null space of Q_i for $i = 1, 2$. In regard of the equation under consideration,

$$\mathcal{N}([\mathbb{E}_{b_ib_i}^{1/2}]^{\dagger}) \subseteq \mathcal{N}(\mathbb{E}_{xb_i}[\mathbb{E}_{b_ib_i}^{1/2}]^{\dagger}). \tag{49}$$

The definition of T_{η_i} implies that $\mathcal{N}(\mathbb{E}_{xb_i}[\mathbb{E}_{b_ib_i}^{1/2}]^{\dagger}) \subseteq \mathcal{N}(T_{\eta_i})$. Therefore (46) follows from (47). As a result, (45) is true. Hence, the statements (34)–(35) are true as well. □

Remark 4 *An estimate of covariance matrices represents a specific problem which is not a topic of this paper. In particular, the expectations and covariance matrices in Lemma* 3 *can be estimated by the techniques developed, for example, by Perlovsky and Marzetta* (1992), *Delmas* (1999), *Kauermann and Carroll* (2001), *Smith and Kohn* (2002), *Conte, De Mario and Ricci* (2002), *Schneider and Willsky* (2003), *Kubokawa and Srivastava* (to appear), *and Leung and Ng (to appear).*

Theorem 1 *The solution to the problem* (18)–(21) *is given by the relations* (9), (25) *and* (33)–(35). *The estimate of* $\mathbf{x}$ *by the estimator* $\hat{\mathcal{P}}$,

$$\hat{\mathbf{x}} = \hat{\mathcal{P}}(\mathbf{y}), \tag{50}$$

estimates $\mathbf{x}$ *with the accuracy represented by*

$$E[\|\mathbf{x} - \hat{\mathcal{P}}(\mathbf{y})\|^2] = \|\mathbb{E}_{xx}^{1/2}\|^2 - \sum_{i=1}^{s} \left[\|\mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}\|^2 - \sum_{j=\eta_i+1}^{p_i} \sigma_{ij}^2 \right]. \tag{51}$$

Proof: It follows from (33)–(43) that

$$E[\|\mathbf{x} - \hat{\mathcal{P}}(\mathbf{y})\|^2] = \|\mathbb{E}_{xx}^{1/2}\|^2 - \sum_{i=1}^{s} \|\mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}\|^2 + \sum_{i=1}^{s} \|U_i D_i V_i^T - T_{\eta_i}\|^2,$$

where (Golub and Van Loan 1996)

$$\|U_i D_i V_i^T - T_{\eta_i}\|^2 = \sum_{j=\eta_i+1}^{p_i} \sigma_{ij}^2$$

for each $i = 1, \ldots, s$. Thus, (51) is true. □

2.2.3 Principal components determination

As for PCA, the proposed estimator $\hat{\mathcal{P}}$ can be represented as a composition of two transforms. One of them is to determine the 'principal components' of the reference vector from the observed data, and the other transform restores the vector.

To show this let us put

$$T_{\eta_i}^{(1)} = U_{\eta_i} D_{\eta_i} \in \mathbb{R}^{m \times \eta_i}, \quad T_{\eta_i}^{(2)} = V_{\eta_i}^T (\mathbb{E}_{b_ib_i}^{1/2})^{\dagger} \in \mathbb{R}^{\eta_i \times n_i} \quad \text{and} \quad M_i = \mathbb{O},$$

where η_i is the rank defined by (21).

We define $\mathcal{T}_{\eta_i}^{(1)}$ and $\mathcal{T}_{\eta_i}^{(2)}$ by the equations

$$[\mathcal{T}_{\eta_i}^{(1)}(\mathbf{c}_i)](\omega) = T_{\eta_i}^{(1)}[\mathbf{c}_i(\omega)] \quad \text{and} \quad [\mathcal{T}_{\eta_i}^{(2)}(\mathbf{b}_i)](\omega) = T_{\eta_i}^{(2)}[\mathbf{b}_i(\omega)]$$

respectively, where $\mathbf{c}_i = \mathcal{T}_{\eta_i}^{(2)}(\mathbf{b}_i)$ and $i = 1, \ldots, s$.

Then the proposed estimator $\hat{\mathcal{P}}$, given by (18), (33)–(35), can be represented as

$$\hat{\mathcal{P}}(\mathbf{y}) = \hat{q} + \sum_{i=1}^{s} \mathcal{T}_{\eta_i}^{(1)} \mathcal{T}_{\eta_i}^{(2)}(\mathbf{b}_i). \tag{52}$$

Here, $\mathbf{c}_i \in L^2(\Omega, \mathbb{R}^{\eta_i})$ represents the 'principal components' for $\mathbf{b}_i \in L^2(\Omega, \mathbb{R}^{n_i})$ and, consequently, for $\mathbf{z}_i \in L^2(\Omega, \mathbb{R}^{n_i})$ with $\eta_i \leq n_i$.

The vector estimate $\hat{\mathbf{x}}$ and the estimator $\hat{\mathcal{P}}$ can now be written as

$$\hat{\mathbf{x}} = \hat{\mathcal{P}}(\mathbf{y}) = \mathcal{T}^{(1)} \mathcal{T}^{(2)}(\mathbf{y}), \tag{53}$$

where $\mathcal{T}^{(1)}$ and $\mathcal{T}^{(2)}$ are such that

$$\mathcal{T}^{(2)}(\mathbf{y}) = (\mathbf{c}_1, \ldots, \mathbf{c}_s) \tag{54}$$

and

$$\hat{\mathbf{x}} = \mathcal{T}^{(1)}(\mathbf{c}_1, \ldots, \mathbf{c}_s) \tag{55}$$

Hence, $\mathcal{T}^{(2)}$ is the transfrom which determines the vector of principal components $(\mathbf{c}_1, \ldots, \mathbf{c}_s)$, and $\mathcal{T}^{(1)}$ is the transform which restores the vector $\mathbf{x}$ from the data $\mathbf{y}$ in the form $\hat{\mathbf{x}}$.

2.2.4 Summary of the method

In summary, the proposed procedure of estimating the vector $\mathbf{x}$ from noisy data $\mathbf{y}$ consists of the following steps.

1. Partition $\mathbf{y}$ into $\mathbf{z}_1$, ..., $\mathbf{z}_s$ as in (9).
2. Transform $\mathbf{z}_1$, ..., $\mathbf{z}_s$ to $\mathbf{b}_1$, ..., $\mathbf{b}_s$ by (25).
3. Determine $\hat{q}$ and $\hat{\mathcal{A}}_1$, ..., $\hat{\mathcal{A}}_s$ by (33)–(35).
4. Determine the estimate $\hat{\mathbf{x}}$ by (50) with $\hat{\mathcal{P}}$ defined by (18), (33)–(35).
5. Determine the principal components by (54).

In the next sections, we analyse the advantages associated with this approach.

2.3 Comparison with PCA

We compare the proposed method and PCA in relation to the three parameters which are the associated error, compression ratio and computational work.

2.3.1 Associated errors

PCA in terms of the pseudo-inverse operators follows from (9), (25), (33) and (34)–(35) if $s = 1$ (i.e. $\mathcal{C} = \mathcal{C}_1 = I$), $\mathcal{B}_1 = I$, $q = \mathbb{O}$ and $\mathcal{M}_1 = \mathbb{O}$.

The error associated with PCA follows from (51) as a particular case and has the form

$$E[||\mathbf{x} - \mathcal{P}^0(\mathbf{y})||^2] = ||E_{xx}^{1/2}||^2 - \left[||E_{xy}(E_{yy}^{\dagger})^{1/2}||^2 - \sum_{j=\eta+1}^{p} \sigma_j^2 \right], \tag{56}$$

where $\sigma_1, \ldots, \sigma_n$ are singular values of the matrix $E_{xy}(E_{yy}^{\dagger})^{1/2}$ such that $\sigma_1 \geq \cdots \geq \sigma_p > 0$ and $\sigma_{p+1} = \cdots = \sigma_n = 0$.

A comparison of (51) and (56) implies that the error associated with the proposed method is less than the error associated with PCA,

$$E[||\mathbf{x} - \hat{\mathcal{P}}(\mathbf{y})||^2] < E[||\mathbf{x} - \mathcal{P}^0(\mathbf{y})||^2],$$

if

$$\begin{aligned} &|| \mathbb{E}_{xx}^{1/2}||^2 + \sum_{i=1}^{s} \sum_{j=\eta_i+1}^{p_i} \sigma_{ij}^2 - \sum_{i=1}^{s} ||\mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}||^2 \\ &< \ ||E_{xx}^{1/2}||^2 + \sum_{j=\eta+1}^{p} \sigma_j^2 - ||E_{xy}(E_{yy}^{\dagger})^{1/2}||^2. \end{aligned} \tag{57}$$

The distinctions on both sides of (57) are implied by the form of covariance matrices defined by operators $\mathbb{E}$ and E (defined previously in (2) and (16)), orthogonality of vectors $\mathbf{v}_1, \ldots, \mathbf{v}_s$ and their number s, ranks $\eta_1, \ldots, \eta_s$ and η, numbers $p_1, \ldots, p_s$ and p. It follows from (51) that varying s implies a variation in the lefthand side quantity in (57).

In the numerical comparison, presented in Section 3, the error associated with the proposed method (51) is less than the error associated with PCA from 4.5 to 347 times (dependingly on the types of data) for the same or lesser compression ratio and the lesser computational work.

2.3.2 Compression ratios

The lesser a compression ratio is the more effective compression is achieved.

The compression ratio of the proposed method is given by

$$\xi = \frac{1}{n} \sum_{i=1}^{s} \eta_i. \tag{58}$$

It follows from (8) and (58) that

$$\xi < \kappa \quad \text{if} \quad \sum_{i=1}^{s} \eta_i < \eta \tag{59}$$

where κ is the compresion ratio of PCA.

In particular, it follows from the results of simulations, given in Section 3, that for the same or lesser compression ratio, the error and computational work associated with the proposed method are less than those by PCA.

2.3.3 Computational works

As it has been mentioned in Section 1.2, the computational work by PCA-like methods is estimated by $W_{PCA} = \mathcal{O}(mn^2 + n^3)$ flops which is mainly conditioned by the SVD evaluation for the $m \times n$ and $n \times n$ matrices $E_{xy}(E_{yy}^{\dagger})^{1/2}$ and E_{yy}, respectively. The proposed method reduces such a computation to the evaluation of the SVD for s smaller $m \times n_i$ and $n_i \times n_i$ matrices $\mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}$ and $\mathbb{E}_{b_ib_i}$, respectively, with $i = 1, \ldots, s$ and $n_1 + \ldots + n_s = n$. As a result, its computational work is estimated by $W = \mathcal{O}(\sum_{i=1}^{s}(mn_i^2 + n_i^3))$ flops.

For instance, if $m = n$ and $n_i = q$ for all $i = 1, \ldots, s$ then $n = sq$ and $W = \mathcal{O}(\sum_{i=1}^{s}(mn_i^2 + n_i^3)) = \mathcal{O}(2sq^3)$ while $W_{PCA} = \mathcal{O}(mn^2 + n^3) = \mathcal{O}(2s^3q^3)$. That is, in terms of $\mathcal{O}(\cdot)$, our method is $\mathcal{O}(s^2)$ times faster than PCA. However, the estimate $\mathcal{O}(s^2)$ is somewhat unsatisfactory because a constant, associated with the estimate by $\mathcal{O}(\cdot)$, can be comparable with $1/s^2$. In particular, our numerical experiments in Section 3 show that, for some particular data, our method is from 1.8 to 3.8 times faster than PCA for $s = 2, 4, 8$. See Tables 1–3 in this regard. It is worthwhile to note that such smaller computational work gives an accuracy which is from 6 to 347 times better than that of PCA. It is natural that, for accuracy similar to that of PCA, our method requires even lesser computational work.

In practice, the related computational works can be tested for the particular data under consideration.

2.4 Particular case: unconstrained vector estimation

If $\eta = \min\{m, n\}$ in (5), then (7) is the full-rank minimization problem, and the constraint (7) can be omitted. Such an unconstrained particular case represents an important problem in its own right which has been studied, in particular, by Sorenson (1980), Scharf (1991a,b), and Hua and Liu (1998).

The estimator associated with the full-rank minimization problem is often treated as a Wiener-like filter.

A related particular case of the problem (18)–(21) with $\eta_i = \min\{m, n_i\}$ for all $i = 1, \ldots, s$ generalises the full rank estimation problem considered by Sorenson (1980), Scharf (1991a,b), and Hua and Liu (1998). In such a case, the constraint (21) can be omitted, as well as in (5) and (7), so that we consider the relations (18)–(20) only. We write

$$J(q^*, \mathcal{A}_1^*, \ldots, \mathcal{A}_s^*) = \min_{\mathbf{q}, \mathcal{A}_1, \ldots, \mathcal{A}_s} J(q, \mathcal{A}_1, \ldots, \mathcal{A}_s). \tag{60}$$

In other words, $q^*, \mathcal{A}_1^*, \ldots, \mathcal{A}_s^*$ give the unconstrained minimum to $J(q, \mathcal{A}_1, \ldots, \mathcal{A}_s)$.

The unconstrained estimator, defined by $\mathcal{C}$, $\hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s$, q^*, $\mathcal{A}_1^*$, …, $\mathcal{A}_s^*$, is denoted by $\mathcal{P}^*$. We wish to show that $\mathcal{P}^*$ possesses certain advantages over the known full-rank estimators.

Theorem 2 *The solution to the unconstrained problem* (18)–(20) *is given by the operators* $\mathcal{C}$, $\hat{\mathcal{B}}_1, \ldots, \hat{\mathcal{B}}_s$ *given by* (9), (25) *and by the relations*

$$q^* = E[\mathbf{x}] - \sum_{i=1}^{s} A_i^* E[\mathbf{b}_i] \tag{61}$$

and

$$\mathcal{A}_1^* = \mathcal{E}_{xb_i} \mathcal{E}_{b_1 b_1}^{\dagger} + \mathcal{M}_1^* (\mathcal{I} - \mathcal{E}_{b_1 b_1} \mathcal{E}_{b_1 b_1}^{\dagger}), \tag{62}$$

$$\vdots$$

$$\mathcal{A}_s^* = \mathcal{E}_{xb_i} \mathcal{E}_{b_s b_s}^{\dagger} + \mathcal{M}_s^* (\mathcal{I} - \mathcal{E}_{b_s b_s} \mathcal{E}_{b_s b_s}^{\dagger}), \tag{63}$$

where $\mathcal{M}_i^*$ *is the arbitrary operator defin ed similarly to* $\mathcal{M}_i$ *in Lemma 3. The estimate of* $\mathbf{x}$ *by the estimator* $\mathcal{P}^*$,

$$\mathbf{x}^* = \mathcal{P}^*(\mathbf{y}), \tag{64}$$

has an accuracy represented by

$$E[||\mathbf{x} - \mathcal{P}^*(\mathbf{y})||^2] = ||\mathbb{E}_{xx}^{1/2}||^2 - \sum_{i=1}^{s} ||\mathbb{E}_{xb_i} (\mathbb{E}_{b_i b_i}^{\dagger})^{1/2}||^2. \tag{65}$$

Proof: The equations (61)–(63) and (65) follow directly from (43) on the basis of Lemma 1. □

Despite a formal similiarity of Theorem 2 above and Theorem 1 by Torokhti and Howlett (2002), the proposed estimator $\mathcal{P}^*$ and that by Torokhti and Howlett (2002) are different. See Remark 2 in this regard.

Remark 5 *We observe that that the estimate of the error* $E[||\mathbf{x}-\mathcal{P}^*(\mathbf{y})||^2]$ *associated with the proposed estimator* $\mathcal{P}^*$ *is diminished if the quantity* $\sum_{i=1}^{s} ||\mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}||^2$ *is increased.*

2.4.1 Comparison with the known full-rank estimators

The accuracy associated with the estimator $\tilde{\mathcal{P}}$ by Sorenson (1980), Scharf (1991a,b), and Hua and Liu (1998) is represented by the relation

$$E[||\mathbf{x}-\tilde{\mathcal{P}}(\mathbf{y})||^2] = ||E_{xx}^{1/2}||^2 - ||E_{xy}(E_{yy}^{\dagger})^{1/2}||^2, \tag{66}$$

which follows from (65) as a particular case when $s=1$ and $q=\mathbb{O}$. Thus,

$$E[||\mathbf{x}-\mathcal{P}^*(\mathbf{y})||^2] < E[||\mathbf{x}-\tilde{\mathcal{P}}(\mathbf{y})||^2]$$

if

$$||\mathbb{E}_{xx}^{1/2}||^2 - \sum_{i=1}^{s} ||\mathbb{E}_{xb_i}(\mathbb{E}_{b_ib_i}^{\dagger})^{1/2}||^2 < ||E_{xx}^{1/2}||^2 - ||E_{xy}(E_{yy}^{\dagger})^{1/2}||^2. \tag{67}$$

The computational work of the estimator $\mathcal{P}^*$ is estimated to be $\mathcal{O}(\sum_{i=1}^{s}(mn_i^2+n_i^3))$ flops while the computational work of the unconstrained estimators of Sorenson (1980), Scharf (1991a,b), and Hua and Liu (1998) is estimated to be $\mathcal{O}(mn^2+n^3)$ flops. Therefore, the comparative analysis for the case of unconstrained estimators is similar to that given in Section 2.3.3 for the constrained estimators.

3 Numerical results

In this section, we present results of numerical simulations. In particular, we compare the estimators, which follow from our approach, with PCA (Section 3.1), the partitioned PCA by Remark 1 (Section 3.2) and the known unconstrained estimators (Section 3.3).

3.1 Comparison with the PCA

Here, we compare the proposed estimator $\hat{\mathcal{P}}$ and PCA with respect to the three parameters discussed in Section 2.3. They are the associated accuracy, compression ratio and computational work. We choose different types of reference vectors and different types of noisy observed data.

Table 1. Comparison with the PCA

Observed data $Y_{ij}^{(p)} = 50X_{ij}^{(p)}Q_{ij}$									
		Our estimator with $s = 8$			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	1/2	7.3e+06	6.3e+06	1/2	2.0e+07	1.9e+07	3.0	10
64	256	1/2	1.9e+07	1.1e+07	1/2	2.0e+08	2.2e+07	2.1	12
32	64	1/2	2.5e+06	8.0e+06	1/2	2.4e+07	2.4e+07	3.0	10
		Our estimator with $s = 4$			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
32	64	1/2	2.2e+06	9.6e+05	1/2	2.4e+07	2.4e+06	2.5	11
32	64	1/8	0.3e+07	9.4e+05	31/32	2.4e+07	2.4e+06	2.6	8
64	128	1/2	7.7e+06	7.2e+06	1/2	8.0e+07	1.9e+07	2.6	10
64	128	1/16	1.0e+07	7.4e+06	63/64	8.2e+07	2.0e+07	2.7	6
		Our estimator with $s = 2$			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
32	64	1/2	1.8e+06	1.4e+06	1/2	2.6e+07	2.4e+06	1.9	9.1
64	128	1/2	0.8e+07	1.1e+07	1/2	7.1e+07	2.0e+07	1.9	8.7

Table 2. Comparison with the PCA

Observed data $Y_{ij}^{(p)} = X_{ij}^{(p)} + 200Q_{ij}$									
		Our estimator with $s = 8$			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
32	256	1/2	0.1e+08	2.5e+06	1/2	1.2e+08	3.9e+06	1.6	9.6
64	128	1/2	0.6e+07	6.7e+06	1/2	7.8e+07	2.0e+07	3.2	13.0
32	64	1/2	1.8e+06	8.7e+05	1/2	2.7e+07	2.6e+06	3.2	15
		Our estimator with $s = 4$			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
32	256	1/2	0.2e+08	2.5e+06	1/2	1.2e+08	3.9e+06	1.5	11
64	128	1/2	5.8e+06	7.5e+06	1/2	7.9e+07	2.0e+07	2.7	13

In Tables 1 and 2, $X^{(p)} \in \mathbb{R}^{256\times256}$ represents the data obtained from an aerial photograph of a plant[1]. The subscript "p" is associated with the word "plant". We divide $X^{(p)}$ into $m\times\nu$ submatrices $X_{ij}^{(p)} \in \mathbb{R}^{m\times\nu}$ with $i = 1,\ldots,256/m$ and $j = 1,\ldots,256/\nu$. Each submatrix $X_{ij}^{(p)}$ is interpreted as ν

[1]The database is available in http://sipi.usc.edu/services/database/Database.html

realizations of a random vector $\mathbf{x} \in L^2(\Omega, \mathbb{R}^m)$ with a column representing a realization. For $i = 1, \ldots, 256/m$ and $j = 1, \ldots, 256/\nu$, observed data are modeled in the form

$$Y_{ij}^{(p)} = 50 X_{ij}^{(p)} Q_{ij} \quad \text{and} \quad Y_{ij}^{(p)} = X_{ij}^{(p)} + 200 Q_{ij},$$

where Q_{ij} is a matrix with normally distributed entries with mean 0 and variance 1. The term Q_{ij} models noise.

Table 3. Comparison with the PCA

Observed data $Y_{ij}^{(t)} = 30 X_{ij}^{(t)} R_{ij} + 500 Q_{ij} X_{ij}^{(t)}$									
		Our estimator with $s = 8$			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	1/2	3.0e+06	6.4e+06	1/2	1.8e+08	1.9e+07	2.9	58
		Our estimator with s=4			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
32	64	1/2	5.1e+05	9.4e+05	1/2	8.1e+07	2.4e+06	2.6	158
32	64	1/8	3.5e+06	9.5e+05	31/32	8.4e+07	2.5e+06	2.6	24
64	128	1/2	1.4e+06	7.4e+06	1/2	1.8e+08	1.9e+07	2.6	131
64	128	1/16	1.3e+07	7.3e+06	63/64	1.9e+08	1.9e+07	2.6	14
		Our estimator with $s = 2$			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
32	64	1/2	2.5e+05	1.3e+06	1/2	8.6e+07	2.4e+06	1.8	347
64	128	1/2	6.3e+05	1.0e+07	1/2	1.8e+08	1.9e+08	1.9	293
64	128	1/32	1.4e+07	1.1e+07	63/64	1.8e+08	1.9e+08	1.8	12.7

In Table 3, $X^{(t)} \in \mathbb{R}^{256 \times 256}$ represents the data "tree"[1] with the subscript "t" denoting the word "tree". As above, $X^{(t)}$ has been represented by a set of submatrices $X_{ij}^{(t)} \in \mathbb{R}^{m \times \nu}$. Observed data are modeled by

$$Y_{ij}^{(t)} = 30 X_{ij}^{(t)} R_{ij} + 500 Q_{ij} X_{ij}^{(t)}$$

where R_{ij} is a matrix with uniformly distributed entries.

In Tables 1–3,

$$\epsilon_1 = \max_{ij} \|X_{ij} - \hat{P}_{ij}(Y_{ij})\|^2 \quad \text{and} \quad \epsilon_2 = \max_{ij} \|X_{ij} - P_{ij}^0(Y_{ij})\|^2$$

where $X_{ij} = X_{ij}^{(p)}$ or $X_{ij} = X_{ij}^{(t)}$, and $Y_{ij} = Y_{ij}^{(p)}$ or $Y_{ij} = Y_{ij}^{(t)}$, and where $\hat{P}_{ij}$ and P^0 denote matrices associated with the proposed estimator and

PCA, respectively. "CR" means the compression ratio, F_1 and F_2 denote total numbers of flops used by $\hat{P}_{ij}$ and P^0_{ij}, correspondingly, evaluated for all $i = 1, \ldots, 256/m$ and $j = 1, \ldots, 256/\nu$.

It follows from Tables 1–3 that:

(i) the accuracy of the proposed estimator is from 6 to 347 times better than the accuracy of PCA, while

(ii) the number of flops used by the proposed estimator $\hat{P}_{ij}$, F_1, is from 1.5 to 3.2 times less than the number of flops used by PCA, F_2, and

(iii) the compression ratio of the estimator $\hat{P}_{ij}$ is the same as that of PCA or up to $63/2 \approx 31.5$ times better (see the last row in Table 3).

3.2 Comparison with the partitioned PCA

In Remark 1, we mention that an application of PCA to both partitioned vector $\mathbf{x}$ and partitioned data $\mathbf{y}$ leads to the problem which is equivalent to that given by (5) but written in the different notation. At the same time, it is natural to expect that the partitioned PCA possesses certain advantages over PCA applied to $\mathbf{x}$ and $\mathbf{y}$ directly (without a partition of $\mathbf{x}$ and $\mathbf{y}$). In this regard, it is interesting to compare the partitioned PCA and the proposed estimator.

Table 4. Comparison with the partitioned PCA

Observed data $Y_{ij}^{(p)} = 50X_{ij}^{(p)}R_{ij} + 100R_{ij}X_{ij}^{(p)}$											
Our estimator with $s = 8$					Partitioned PCA						
m	ν	CR	Error, ϵ_1	Flops, F_1	m	ν	CR	Error, ϵ_2	Flops, F_2	$\frac{F_2}{F_1}$	$\frac{\epsilon_2}{\epsilon_1}$
64	128	1/2	2.4e+06	6.4e+06	8	128	1/2	1.4e+07	4.2e+08	66.5	6.1
64	256	1/2	6.5e+06	1.0e+07	8	256	1/2	2.9e+07	4.8e+08	45.3	4.5
32	64	1/2	8.1e+05	8.3e+05	4	64	1/2	6.4e+06	5.6e+07	70.0	7.8
Our estimator with $s = 4$					Partitioned PCA						
m	ν	CR	Error, ϵ_1	Flops, F_1	m	ν	CR	Error, ϵ_2	Flops, F_2	$\frac{F_2}{F_1}$	$\frac{\epsilon_2}{\epsilon_1}$
32	64	1/2	6.5e+05	9.5e+05	8	64	1/2	1.2e+07	1.6e+07	16.9	18.9
32	64	1/8	1.7e+06	9.5e+05	8	64	1/8	1.4e+07	1.6e+07	17.2	7.9
64	128	1/2	1.6e+06	7.3e+06	16	128	1/2	2.7e+07	1.3e+08	17.2	16.9
64	128	1/16	9.6e+06	7.3e+06	16	128	1/16	3.0e+07	1.3e+08	17.3	3.1
Our estimator with $s = 2$					Partitioned PCA						
m	ν	CR	Error, ϵ_1	Flops, F_1	m	ν	CR	Error, ϵ_2	Flops, F_2	$\frac{F_2}{F_1}$	$\frac{\epsilon_2}{\epsilon_1}$
32	64	1/2	4.9e+05	1.3e+06	16	64	1/2	2.3e+07	5.5e+06	4.2	46.8
64	128	1/2	1.1e+06	1.0e+07	32	128	1/2	4.9e+07	4.2e+07	4.1	44.5
128	256	1/2	3.1e+06	7.9e+07	64	256	1/2	1.5e+08	3.3e+08	4.2	49.4

Table 5. Comparison with the partitioned PCA

Observed data $Y_{ij}^{(t)} = 30X_{ij}^{(t)}R_{ij} + 500Q_{ij}X_{ij}^{(t)}$											
Our estimator with $s = 8$					Partitioned PCA						
m	ν	CR	Error, ϵ_1	Flops, F_1	m	ν	CR	Error, ϵ_2	Flops, F_2	$\frac{F_2}{F_1}$	$\frac{\epsilon_2}{\epsilon_1}$
128	256	1/2	8.8e+6	5.0e+07	16	256	1/2	1.3e+08	3.2e+09	65	15
64	128	1/2	2.7e+6	6.6e+06	8	128	1/2	4.0e+07	4.2e+08	65	15
Our estimator with $s = 4$					Partitioned PCA						
m	ν	CR	Error, ϵ_1	Flops, F_1	m	ν	CR	Error, ϵ_2	Flops, F_2	$\frac{F_2}{F_1}$	$\frac{\epsilon_2}{\epsilon_1}$
128	256	1/2	4.8e+06	5.8e+07	32	256	1/2	2.4e+08	9.4e+08	16.3	50
Our estimator with $s = 2$					Partitioned PCA						
m	ν	CR	Error, ϵ_1	Flops, F_1	m	ν	CR	Error, ϵ_2	Flops, F_2	$\frac{F_2}{F_1}$	$\frac{\epsilon_2}{\epsilon_1}$
64	128	1/2	6.5e+05	1.0e+07	32	128	1/2	1.3e+08	4.1e+08	4.0	195

In Tables 4 and 5, we present the numerical results of random vector esimates given by matrices $X_{ij}^{(p)}$ (Table 4) and $X_{ij}^{(t)}$ (Table 5) with

$$Y_{ij}^{(p)} = 50X_{ij}^{(p)}R_{ij} + 100R_{ij}X_{ij}^{(p)} \quad \text{and} \quad Y_{ij}^{(t)} = 30X_{ij}^{(t)}R_{ij} + 500Q_{ij}X_{ij}^{(t)},$$

respectively.

We observe that:

(i) the accuracy of the proposed estimator is from 3.1 to 195 times better than the accuracy of the partitioned PCA, and

(ii) the number of flops F_1 used by the proposed estimator $\hat{P}_{ij}$ is from 4.1 to 70 times less than the number of flops F_2 used by the partitioned PCA, while

(iii) the compression ratio of the estimator $\hat{P}_{ij}$ is the same as that of the partitioned PCA.

3.3 Comparison with the known unconstrained estimators

In this Section, we present the numerical results for the proposed unconstrained estimator $\mathcal{P}^*$ and unconstrained estimators by Sorenson (1980), Scharf (1991a,b), and Hua and Liu (1998), which are denoted as "Known estimators".

In Tables 6–8, we use the same data as for the constrained esimators in Section 3.1. In Table 9, the observed data are simulated by matrix $Y_{ij}^{(t)} = X_{ij}^{(t)} \bullet X_{ij}^{(t)}$ where the symbol "$\bullet$" denotes the Hadamard matrix product.

The presented results demonstrate that:

(i) the accuracy of the proposed estimator $\mathcal{P}^*$ is from 3.6 to $3.0e{+}18$ times better than the accuracy of the known unconstrained estimators, while

(ii) the number of flops F_1 used by the proposed estimator $\hat{P}_{ij}$ is from 1.1 to 2.0 times less than the number of flops F_2 used by the known unconstrained estimators.

Table 6. Comparison with the known unconstrained estimators

Observed data $Y_{ij}^{(p)} = 50X_{ij}^{(p)}Q_{ij}$							
		Our estimator with $s = 8$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	0.7e+07	5.9e+06	7.3e+07	8.6e+06	1.5	11
64	256	1.7e+07	1.1e+07	1.9e+08	1.2e+07	1.1	11
64	64	1.6e-11	3.2e+06	3.7e+06	6.4e+06	2.0	2.3e+17
		Our estimator with $s = 4$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
32	64	0.2e+07	7.9e+05	2.4e+07	1.1e+06	1.3	9.8
64	128	7.1e+06	6.2e+06	8.2e+07	8.4e+06	1.4	11
128	128	9.0e-13	2.8e+07	2.8e+06	5.1e+07	1.8	3.0e+18
		Our estimator with $s = 2$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	0.8e+07	7.0e+06	7.1e+07	8.5e+06	1.2	8.9
32	64	0.2e+07	7.7e+05	2.5e+07	1.1e+06	1.4	12
32	32	3.5e-11	5.9e+05	2.8e+06	8.2e+06	1.4	8.0e+16

Table 7. Comparison with the known unconstrained estimators

Observed data $Y_{ij}^{(p)} = X_{ij}^{(p)} + 200Q_{ij}$							
		Our estimator with $s = 8$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	256	1.4e+07	1.1e+07	2.1e+08	1.3e+07	1.1	15
64	128	0.5e+07	5.9e+07	7.6e+07	9.3e+07	1.6	14
32	64	1.6e+06	7.8e+05	3.0e+07	1.2e+06	1.6	19
		Our estimator with $s = 4$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	256	1.4e+07	1.1e+07	2.1e+08	1.3e+07	1.1	15
64	128	5.3e+06	6.3e+06	7.8e+07	9.3e+06	1.5	14
32	64	1.7e+06	8.1e+05	2.7e+07	1.2e+06	1.5	16
		Our estimator with $s = 2$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	5.1e+06	7.4e+06	7.8e+07	9.5e+07	1.3	15
32	64	1.5e+06	9.6e+05	2.7e+07	1.2e+06	1.2	17

Table 8. Comparison with the known unconstrained estimators

Observed data $Y_{ij}^{(t)} = 30X_{ij}^{(t)}R_{ij} + 500Q_{ij}\tilde{X}_{ij}^{(t)}$							
		Our estimator for $s = 8$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	2.5e+04	5.9e+06	1.8e+08	8.4e+06	1.4	7.2e+03
32	64	1.1e+04	7.7e+05	8.2e+07	1.1e+06	1.4	7.7e+03
		Our estimator for $s = 4$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	3.0e+04	6.2e+06	1.8e+08	8.4e+06	1.4	6.1e+03
32	64	1.1e+04	8.0e+05	9.0e+07	1.1e+06	1.3	8.4e+03
		Our estimator for $s = 2$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	2.4e+04	7.0e+06	1.9e+08	8.4e+06	1.2	7.7e+03
32	64	1.5e+04	9.1e+05	8.5e+07	1.1e+06	1.2	5.8e+03

The presented results demonstrate that:

(i) the accuracy of the proposed estimator $\mathcal{P}^*$ is from 3.6 to $3.0e+18$ times better than the accuracy of the known unconstrained estimators, while

(ii) the number of flops F_1 used by the proposed estimator $\hat{P}_{ij}$ is from 1.1 to 2.0 times less than the number of flops F_2 used by the known unconstrained estimators.

Table 9. Comparison with the known unconstrained estimators

Observed data $Y_{ij}^{(t)} = X_{ij}^{(t)} \bullet X_{ij}^{(t)}$							
		Our estimator for $s = 8$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	0.9e+05	5.9e+06	3.3e+08	8.4e+06	1.4	3.6
32	64	0.4e+05	7.7e+05	1.9e+05	1.1e+06	1.4	4.5
64	64	4.7e-13	3.2e+06	5.7e+03	6.5e+05	2.0	1.2e+15
32	32	7.3e-15	4.2e+05	5.8e+03	8.4e+05	2.0	8.0e+16
		Our estimator for $s = 4$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	0.9e+05	6.1e+06	3.3e+08	8.4e+06	1.4	3.6
128	128	9.0e-12	2.8e+07	1.6e+03	5.3e+07	1.9	1.8e+14
64	64	5.7e-14	3.4e+06	5.7e+03	6.5e+05	1.8	9.9e+15
		Our estimator for $s = 2$		Known estimators			
m	ν	Error, ϵ_1	Flops, F_1	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
64	128	0.9e+05	7.0e+06	3.3e+05	8.4e+06	1.2	3.6
64	64	6.1e-11	4.5e+06	5.7e+03	6.5e+06	1.4	9.4e+14
32	32	6.4e-16	5.9e+05	5.8e+03	8.4e+05	1.4	9.2e+17

4 Discussion of results

As has been discussed above, the proposed approach leads to advantages over PCA in relation to the associated accuracy, compression ratio and computational work.

One should note that these advantages are not unconditional: they are achieved if condition (57) is true. Thus, in practical computations, condition (57) should be verified first.

In the following examples, we show how the data parameters influence on performance of the proposed estimators $\hat{\mathcal{P}}$ and $\mathcal{P}^*$.

Table 10

Observed data $Y_{ij}^{(p)} = X_{ij}^{(p)} + 200Q_{ij}$									
		Our estimator with $s = 4$			PCA				
m	ν	CR	Error, ϵ_1	Flops, F_1	CR	Error, ϵ_2	Flops, F_2	F_2/F_1	ϵ_2/ϵ_1
128	128	1/2	1.2e+06	4.6e+07	1/2	5.6e+04	1.4e+08	2.9	4.8e-2
64	128	1/2	5.8e+06	7.5e+06	1/2	7.9e+07	2.0e+07	2.7	13

Example 1 *In Table* 7*, we present the results of the applications of the proposed estimator* $\hat{\mathcal{P}}$ *and PCA to data* $Y_{ij}^{(p)}$ *with* $s = 2, 4, 8$*,* $m = 32, 64$ *and* $\nu = 64, 128, 256$*.*

If we apply the proposed estimator $\hat{\mathcal{P}}$ *to the data* $Y_{ij}^{(p)}$ *with* $m = 128$ *(i.e. with 'm' different from that in Table* 7*),* $\nu = 128$ *and* $s = 4$ *then condition* (57) *is not true, and the error associated with the estimator* $\hat{\mathcal{P}}$ *is greater than the error associated with PCA. See the first row in the Table 10 for the corresponding results. Nevertheless, a reduction of* $m = 128$ *to* $m = 64$ *leads to the case when condition* (57) *is true and consequently to the substantial improvement in the accuracy of the estimator* $\hat{\mathcal{P}}$*. See the second row in Table* 10*.*

Table 11

Observed data $Y_{ij}^{(p)} = 50X_{ij}^{(p)}R_{ij} + 100R_{ij}X_{ij}^{(p)}$											
Our estimator with $s = 8$					Partitioned PCA						
m	ν	CR	Error, ϵ_1	Flops, F_1	m	ν	CR	Error, ϵ_2	Flops, F_2	$\frac{F_2}{F_1}$	$\frac{\epsilon_2}{\epsilon_1}$
128	128	1/2	2.2e+06	3.3e+07	16	128	1/2	2.2e+05	3.1e+09	94	0.1
64	128	1/2	2.1e+06	6.4e+06	8	128	1/2	1.4e+07	4.3e+08	67.6	6.5

Example 2 *Let us choose data from Table* 4 *with* $m = 128$ *and* $s = 8$ *which have not been used in Table* 4*. As in Example 1 above, for such a value of* m*, and for* $\nu = 128$ *and* $s = 8$*, condition* (57) *is not true. As a result, the accuracy* ϵ_1 *of the estimator* $\hat{\mathcal{P}}$ *is 10 times less than the accuracy* ϵ_2 *of the partitioned PCA. See the first row in Table* 11*. Nevertheless, a reduction of* $m = 128$ *to* $m = 64$ *leads to a decrease of the left hand side of condition* (57) *so that the latter becomes true. Then* ϵ_1 *becomes 6.5 times less than* ϵ_2*. See the second row in Table* 11*. We also observe that our estimater takes substantially fewer flops than that of PCA.*

The examples demonstrate how the performance of the proposed estimates can be improved by varying the data parameters.

5 Conclusion

A determination of so called 'principal components' from a random vector is an important problem in data analysis. Such a problem can be solved by PCA which produces the optimal *linear* estimator.

The new results obtained in the paper are summarized as follows.

We have proposed and justified the *non-linear* estimator which, under condition (57), can perform better than PCA. While PCA performance is varied due to varying one parameter only (the compression ratio), the performance of our estimator is further improved due to the implementation of the original data partition and the proposed orthogonalisation procedure. It has been shown, that condition (57) is not overly restrictive and, if necessary, it can be overcome by varying the data parameters.

The rigorous analysis of the numerical error associated with the presented method has been given (Section 2.2).

The comparative analysis of the proposed approach with PCA, the partitoned PCA and the known unconstrained estimators has been provided (Sections 2.3, 2.4 and 3).

The differences from the known estimators have also been discussed (Remark 2).

The proposed approach can be extended to the estimators of higher degrees (Yamada, Sekiguchi and Sakaniwa 2000), locally reduced-rank estimators (Yamada and Elbadraoui 2003) and the iterative estimators (Torokhti and Howlett 2003b).

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