On some limitations of probabilistic models for dimension-reduction: illustration in the case of one particular probabilistic formulation of PLS

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**Abstract**

Partial Least Squares (PLS) refer to a class of dimension-reduction techniques aiming at the identification of two sets of components with maximal covariance, in order to model the relationship between two sets of observed variables \(x \in \mathbb{R}^p\) and \(y \in \mathbb{R}^q\), with \(p \geq 1, q \geq 1\). \cite{elBouhaddani} have recently proposed a probabilistic formulation of PLS. Under the constraints they consider for the parameters of their model, this latter can be seen as a probabilistic formulation of one version of PLS, namely the PLS-
SVD. However, we establish that these constraints are too restrictive as they define a very particular subset of distributions for \((x, y)\) under which, roughly speaking, components with maximal covariance (solutions of PLS-SVD), are also necessarily of respective maximal variances (solutions of the principal components analyses of \(x\) and \(y\), respectively). Then, we propose a simple extension of el Bouhaddani et al.’s model, which corresponds to a more general probabilistic formulation of PLS-SVD, and which is no longer restricted to these particular distributions. We present numerical examples to illustrate the limitations of the original model of el Bouhaddani et al. (2017).

**Keywords.** Partial least squares, PLS, probabilistic formulation, identifiability.

1 Introduction

Principal Component Analysis (PCA), Canonical Correlation Analysis (CCA) and Partial Least Squares (PLS) are arguably among the most popular multivariate methods for dimension-reduction. They have been described and applied for many years (Hotelling 1933, 1936; Jöreskog and Wold 1982; Sampson et al. 1989; Wold 1985), but are still the subject of active research and discussion (Abdi et al. 2013; Jolliffe 2002, 2005; Jolliffe and Cadima 2016; Krishnan et al. 2011). Overall, these methods aim at the identification of vectors of weights, from which components are defined as linear transformations of the observed variables. Under each particular method, these weights are chosen so that the corresponding components meet a particular criterion.
For example, given a data matrix $X$ containing $n$ observations of a $p$-variate variable $x$ (with $n \geq 1$, $p \geq 1$), the goal of PCA is to identify $r \leq p$ vectors of weights that define $r$ mutually orthogonal principal components with maximal variances; the matrix of principal components $\mathbf{X} = \mathbf{X}A$ then consists of linear combinations of the $p$ columns of $\mathbf{X}$, with the matrix of weights $A$ given by the eigenvectors associated with the $r$ largest eigenvalues of the sample variance matrix $\mathbf{X}^\top\mathbf{X}$. On the other hand, given two data matrices $\mathbf{X}$ and $\mathbf{Y}$, that gather the $n \geq 1$ observations for a pair of variables $(x, y)$, with $x \in \mathbb{R}^p$ and $y \in \mathbb{R}^q$, $p, q \geq 1$, the goal of CCA and PLS is to model the relationship between $x$ and $y$ by identifying weights that define components with maximal association. Although CCA, which looks for components with maximal correlation, is sometimes considered as a PLS technique, the PLS qualifier usually rather refers to the class of methods that look for components with maximal covariance (Wegelin, 2000). The family of PLS methods still consists of a number of techniques, such as PLS Regression, PLS-W2A or PLS-SVD (Rosipal and Krämer, 2006, Wegelin, 2000). PLS Regression treats the two sets of variables asymmetrically: it focuses on the construction of components from one set of variables, which are then considered as predictors of the second set of variables (the response). On the other hand, both PLS-W2A and PLS-SVD adopt a more symmetrical perspective, and aim at the identification of two sets of weight vectors defining two sets of components. In particular, PLS-SVD, sometimes also referred to as PLS-SB or PLS-C (Krishnan et al., 2011, Sampson et al., 1989, Wegelin, 2000), is simply based on the Singular Value Decomposition (SVD) of the sample covariance matrix $\mathbf{X}^\top\mathbf{Y}$, and defines the two sets of weights as left and right
singular vectors of $X^\top Y$, respectively. For the sake of completeness, we shall recall that, in contrast, both PLS Regression and PLS-W2A are iterative methods, based on a principle called deflation, which is applied iteratively to guarantee some particular orthogonality properties \cite{Hoskuldsson1988, Rosipal2006, Wegelin2000, Wold1985}.

Over the last two decades, several probabilistic formulations of these various dimension-reduction techniques have been introduced, first under a Gaussian setting. They include the Probabilistic PCA (PPCA) \cite{Tipping1999}, the Probabilistic CCA (PCCA) \cite{Bach2005}, as well as several versions of Probabilistic PLS (PPLS) \cite{elBouhaddani2017, Li2015, Zheng2016}. Regarding these three probabilistic formulations of the PLS, both \cite{Zheng2016} and \cite{Li2015} focus on PLS Regression (the model considered by \cite{Li2015} has commonalities with a probabilistic formulation of Principal Component Regression (PCR) \cite{Ge2011}), while \cite{elBouhaddani2017} consider a symmetrical PLS approach. Overall, all these probabilistic formulations rely on structural equations that define the observed variables as linear combinations of some latent variables plus some Gaussian noise. Parameter estimation under these latent variable models is then usually performed via an Expectation-Maximization (EM) algorithm \cite{Dempster1977}. Giving access to all the likelihood-based inference machinery, these probabilistic formulations have a number of advantages compared to their standard formulation counterpart \cite{Rosipal2006, Smilde2004}. The estimation can be computationally more efficient, and can deal with missing data \cite{Tipping1999, Zheng2016}. Moreover, covariates can be included
in the model (Chiquet et al., 2017), and penalized versions of the likelihood can be used to encourage sparsity or structured sparsity, in particular in a high-dimensional framework (Guan and Dy, 2009; Park et al., 2017; Zeng et al., 2017). Finally, the probabilistic formulation is very versatile, and turns several complex settings into natural extensions of the simple Gaussian ones mentioned above. For example, probabilistic PCA models have been proposed for binary data and count data (Chiquet et al., 2017; Durif et al., 2019). Extensions to even more complex settings, including mediation analysis where three sets of observed variables are involved, have also been proposed (Derkach et al., 2019).

To recap, probabilistic formulations of dimension-reduction techniques enjoy a number of appealing properties. However, appearances can be deceptive, and we will show in this article that some caution is needed when developing and applying them. Indeed, despite their apparent ability to fully capture the relationships among the variables under study, some of them manage to do so under very particular distributions only: when constraints on the model parameters are too strong, the parameters of interest reduce to parameters that could be obtained under much more simple models, which greatly limits the applicability and interest of the corresponding models. For illustration, we will focus here on the probabilistic PLS model proposed by el Bouhaddani et al. (2017), which we will simply refer to as the PPLS model from now on. In Section 2.1, we recall the principle of the PPLS model as proposed by el Bouhaddani et al. (2017), and emphasize that it can be regarded as a probabilistic formulation of PLS-SVD. In Section 2.2, we show that this PPLS model suffers from the aforementioned defect, and actually
defines a set of very particular distributions for \((x, y)\), which limits its applicability. We propose a more general probabilistic formulation of PLS-SVD in Section 2.3. In Section 3, we present numerical examples to illustrate the limitations of the original PPLS model of el Bouhaddani et al. (2017). Concluding remarks are finally presented in Section 4.

2 PPLS models

2.1 The original PPLS model proposed by el Bouhaddani et al. (2017)

The PPLS model proposed by el Bouhaddani et al. (2017) is defined by the following structural equations, which relate the two observed sets of variables \(x \in \mathbb{R}^p\) and \(y \in \mathbb{R}^q\) to two sets of latent variables \(t \in \mathbb{R}^r\) and \(u \in \mathbb{R}^r\), with \(r < \min(p, q)\),

\[
x = tW^T + e, \quad y = uC^T + f, \quad u = tB + h.
\]  

el Bouhaddani et al. (2017) imposed the constraints (a)-(i) below on the model parameters to ensure identifiability.

(a) \(t \sim \mathcal{N}(0, \Sigma_t)\).

(b) \(\Sigma_t\) is a \(r \times r\) diagonal matrix, with strictly positive diagonal elements.

(c) \(e \sim \mathcal{N}(0_p, \sigma_e^2 I_p)\). (d) \(f \sim \mathcal{N}(0_q, \sigma_f^2 I_q)\). (e) \(h \sim \mathcal{N}(0_r, \sigma_h^2 I_r)\).

(f) \(W\) and \(C\) are respectively \(p \times r\) and \(q \times r\) semi-orthogonal matrices.
(g) $B$ is a diagonal matrix, with strictly positive diagonal elements.

(h) the diagonal elements of $\Sigma B$ are strictly decreasingly ordered.

(i) $r < \min(p, q)$.

Here $I_p$ denote the identity matrix of size $p \times p$, and $0_p$ the vector $(0, \ldots, 0)$ of size $p$. The parameters of the model are given by $\theta = (W, C, B, \Sigma_t, \sigma^2_e, \sigma^2_f, \sigma^2_h)$. In particular, matrices $W = (W_1, \cdots, W_r)$ and $C = (C_1, \cdots, C_r)$ contain the two sets of weight vectors; note that they are the “true weights”, defined from the theoretical distribution of $(x, y)$. Given estimates $\hat{W}$ and $\hat{C}$ of these quantities, two sets of empirical components can be defined as linear combination of the two sets observed variables. In this work, we will mostly focus on components defined as $\hat{X} = X\hat{W}$ and $\hat{Y} = Y\hat{C}$; we recall that, when working with latent variable models, an alternative strategy consists in using appropriate conditional expectations of the latent variables; see [Bach and Jordan (2005)] and Section 2.3 below for more details. We shall further stress that the latent variables $t$ and $u$ do not directly correspond to the components $x = xW = t + eW$ and $y = yC = u + fC$, even if, in this case, $\text{Cov}(x, y) = \text{Cov}(t, u)$.

Under the constraints (a)-(i), [el Bouhaddani et al. (2017)] establish the identifiability of their model (up to sign for the columns of parameters $W$ and $C$). In particular, observe that $\text{Cov}(x, y) = W\Sigma_t BC^\top$, and recall that $W$ and $C$ are semi-orthogonal matrices, and that $\Sigma_t B$ is diagonal with strictly decreasingly ordered diagonal elements. Then, the first $r$ non-null singular values of $\text{Cov}(x, y)$ are all distinct, and are given by the diagonal of $\Sigma_t B$. As a result, and as established by [el Bouhaddani et al. (2017)], the columns
of $W$ and $C$ are uniquely defined (up to sign) as the first $r$ left and right
singular vectors of $\text{Cov}(x,y)$, respectively. Although they do not mention it,
their model can therefore be regarded as a probabilistic formulation of PLS-
SVD. In particular, this means that the two sets of components $x = xW$ and
$y = yC$ coincide with the two sets of components with maximal covariance,
targeted by the PLS-SVD.

However, we establish in Section 2.2 that the two sets of weights $W$ and
$C$, which are the theoretical solutions of the PPLS model, are also necessarily
the theoretical solutions of two PPCA models for $x$ and $y$, respectively. In
other words, we will see that the PPLS model defines a set of very particular
distributions for $(x,y)$ under which the two sets of components with maximal
covariance, $x = xW$ and $y = yC$, are also necessarily of respective maximal
variances.

2.2 Limitation of the original PPLS model

We show in Appendix A that, under the PPLS model of el Bouhaddani et al.
(2017), the columns of $W$ and $C$ are also eigenvectors corresponding to the
$r$ largest eigenvalues of $\text{Var}(x)$ and $\text{Var}(y)$, respectively. Therefore, under
the PPLS model, the two sets of components $x = xW$ and $y = yC$ are
not only of maximal covariance, but they are also necessarily of respective maximal variances. As shown in Appendix A, this comes from the fact
that under the PPLS model, we also have $\text{Var}(x) = W\Sigma_r W^\top + \sigma_e^2 I_p$, and
$\text{Var}(y) = C(\Sigma_t B^2 + \sigma_h^2 I_r)C^\top + \sigma_f^2 I_q$. Equivalently, it follows from the fact
that the PPLS model implies that both $x$ and $y$ fulfill the following PPCA
model, presented here for a generic observed variable \( z \in \mathbb{R}^d \)

\[
    z = vV^T + g,
\]

under the constraints

(\(\alpha\)) \( v \sim \mathcal{N}(0, \Sigma_V) \).

(\(\beta\)) \( \Sigma_V \) is a \( r \times r \) diagonal matrix, with strictly positive diagonal elements.

(\(\gamma\)) \( g \sim \mathcal{N}(0_d, \sigma_g^2 I_d) \).

(\(\delta\)) \( V \) is a \( d \times r \) semi-orthogonal matrix.

(\(\epsilon\)) \( r < d \).

This PPCA model is a variation of the one introduced by Tipping and Bishop (1999); see Appendix B for more details. First consider this PPCA model for the observed variable \( x \in \mathbb{R}^p \). By comparing, on the one hand, constraints (\(a\)), (\(b\)), (\(c\)), (\(f\)) and (\(i\)) with constraints (\(\alpha\)) – (\(\epsilon\)), and, on the other hand, Equation (2) and the first equation in Equation (1), it appears that the unique solution \( W \) of the PPLS model necessarily corresponds to one of the possibly many solutions \( V \) of this PPCA model for \( x \). More precisely, when the solution of the PPCA model for \( x \) is unique (up to sign), that is when the diagonal elements of \( \Sigma_x \) are all distinct, then the \( r \) largest eigenvalues of \( \text{Var}(x) \) are all of algebraic multiplicity equal to one, the associated eigenvectors are uniquely defined (up to sign), and they correspond to the columns of \( V \). They are also the columns \( W_1, \ldots, W_r \) of \( W \), although not necessarily in the same order; columns of \( W \) and \( V \) are in the same order if, and only if,
the diagonal elements of \( \Sigma_t \) are in decreasing order too. Now, if the diagonal elements of \( \Sigma_t \) are not all distinct, then the solution \( V \) of the PPCA model for \( x \) is not unique, but the columns of \( W \) still necessarily constitute one of these solutions, that is one particular set of eigenvectors corresponding to the \( r \) largest eigenvalues of \( \text{Var}(x) \).

Similarly, the PPLS model implies that the PPCA model above holds for the observed variable \( y \in \mathbb{R}^q \) too, and that the unique solution \( C \) of the PPLS model necessarily corresponds to one of the possible solutions of this PPCA model for \( y \). More precisely, if the diagonal elements of \( \Sigma_t B^2 \) are all distinct, then the columns of \( C \) correspond to the uniquely defined \( r \) eigenvectors associated with the \( r \) largest eigenvalues of \( \text{Var}(y) \). On the other hand, if the diagonal elements of \( \Sigma_t B^2 \) are not all distinct, then the columns of \( C \) still constitute one of the solutions of the PPCA model for \( y \); in particular, they are one of the possible sets of eigenvectors for the \( r \) largest eigenvalues of \( \text{Var}(y) \).

In other words, the PPLS model of el Bouhaddani et al. (2017) corresponds to a model where two PPCA models, one for \( x \) and one for \( y \), are related to each other via the third equation in Equation (1). But then, because the weight matrices \( W \) and \( C \), solutions of their PPLS model, are also necessarily solutions of two PPCA models for \( x \) and \( y \), their model defines a subset of very particular distributions for \( (x, y) \), under which components \( x = xW \) and \( y = yC \) are not only of maximal covariance, but also of respective maximal variances. In particular, if the diagonal elements of \( \Sigma_t \) are all distinct, and if the same holds true for \( \Sigma_t B^2 \), the “solutions” of the two distinct PPCA models are uniquely defined, and then each of the two marginal
distributions of $x$ and $y$ are sufficient to respectively identify each of the two sets of weights that define components with maximal covariance. As will be confirmed in Section 3, this greatly limits its applicability.

2.3 A more general probabilistic formulation of the PLS-SVD

We now present a generalization of the PPLS model of el Bouhaddani et al. (2017), which corrects its main defect and defines a broader set of distributions for $(x, y)$. Our general idea was to keep the same general form as that of el Bouhaddani et al. (2017), but with weaker constraints, in such a way that the weights $W$ and $C$ cannot generally be identified from the marginal distributions of $x$ and $y$ only.

In the PPLS model, assumptions (a)-(i) are related to various aspects of the model: the distributions of the errors terms, the distributions of the latent variables, as well as “direct” constraints on the model parameter $\theta = (W, C, B, \Sigma_t, \sigma^2_e, \sigma^2_f, \sigma^2_h)$. In order to keep the link with the PLS-SVD for our “extended” PPLS model, we still assume that the weights matrices $W$ and $C$ are semi-orthogonal, and that the variance matrices of the latent variables are diagonal. As a start, we thus only relax the constraints (c) and (d) on the isotropy of the variance matrices for the error terms $e$ and $f$, and we simply assume that these variance matrices are positive semi-definite, that is that the error terms $e$ and $f$ are two non-degenerate Gaussian vectors. We will therefore replace constraints (c) and (d) by constraints (c*) and (d*) presented below. But then, to preserve the identifiability of the model (see
below), we have to consider a model with only one set of latent variables, in 
the same vein as the PCCA model of [Bach and Jordan, 2005]. Our extended 
PPLS model is then defined by the following two structural equations

\[ x = tW^\top + e, \quad y = tC^\top + f, \]

(3)

under the constraints (a), (b), (f), (i) and:

(c*) \( e \sim \mathcal{N}(0_p, \Psi_e) \), with \( \Psi_e \) a \( p \times p \) semi-positive definite matrix.

(d*) \( f \sim \mathcal{N}(0_q, \Psi_f) \), with \( \Psi_f \) a \( q \times q \) semi-positive definite matrix.

(h*) the diagonal elements of \( \Sigma_t \) are strictly decreasingly ordered.

Note that condition (h*) is the analogue of condition (h) in the case where 
only one set of latent variables is considered. Further observe that \( \text{Cov}(x, y) = W\Sigma_t C^\top, \text{Var}(x) = W\Sigma_t W^\top + \Psi_e, \) and \( \text{Var}(y) = C\Sigma_t C^\top + \Psi_f, \) where \( \theta = (W, C, \Sigma_t, \Psi_e, \Psi_f) \) are the parameters of our model.

We now present the sketch of the proof of the identifiability of our ex-
tended PPLS model, which is an adaptation of the one developed by [el Bouhad-
dani et al., 2017]; we refer to Appendix C for a more detailed on the proof.

Consider two pairs of random variables, \((x, y)\) and \((\tilde{x}, \tilde{y})\), drawn from two 
extended PPLS models, with respective parameters \( \theta = (W, C, \Sigma_t, \Psi_e, \Psi_f) \)
and \( \tilde{\theta} = (\tilde{W}, \tilde{C}, \tilde{\Sigma}_t, \tilde{\Psi}_e, \tilde{\Psi}_f) \). Let \( \Sigma \) and \( \tilde{\Sigma} \) denote their variance-covariance 
matrices. Now, assume that \( \Sigma = \tilde{\Sigma} \). This is equivalent to
Matrices $W$, $C$, $\tilde{W}$, and $\tilde{C}$ are all semi-orthogonal, and both $\Sigma_t$ and $\tilde{\Sigma}$ are diagonal with strictly decreasing diagonal elements. As detailed in Appendix C, Equation (6) implies that $\Sigma_t = \tilde{\Sigma}_t$, $W = \tilde{W} J$, and $C = \tilde{C} J$, with $J$ a diagonal matrix with $\pm 1$ elements on the diagonal. Then, Equation (4) implies that $\Psi_e = \tilde{\Psi}_e$, while Equation (5) implies that $\Psi_f = \tilde{\Psi}_f$. As a result, the parameters of the extended PPLS model given in Equation (3) are identifiable (up to sign for the columns of $W$ and $C$). In particular, because Cov($x,y$) = $W\Sigma_tC^T$, parameters $W$ and $C$ are identified (up to sign) as the first $r$ left and right singular vectors of Cov($x,y$), respectively.

Moreover, because Var($x$) = $W\Sigma_tW^T + \Psi_e$, and Var($y$) = $C\Sigma_tC^T + \Psi_f$, with $\Psi_e$ and $\Psi_f$ two positive semi-definite matrices, we shall stress that $W$ and $C$ can generally not be identified from the eigendecomposition of Var($x$) and Var($y$), respectively. In other words, the two sets of weights $W$ and $C$ define components with maximal covariance, which are not necessarily of respective maximal variances, and $W$ and $C$ cannot generally be identified separately from the marginal distributions of $x$ and $y$. Our extended PPLS model can therefore be regarded as a more general probabilistic formulation of the PLS-SVD, which defines a much broader and interesting set of distributions than the original PPLS model of el Bouhaddani et al. (2017).
We will now conclude this Section by a few remarks on our model. First, two sets of components can be defined as linear transformations of \( x \) and \( y \), respectively. As above, just as under the standard PLS-SVD (Wegelin, 2000), a first strategy consists in defining \( x = xW \) and \( y = yC \). Following Bach and Jordan (2005), alternative components are defined as \( x^* = E(t|x; \theta) \) and \( y^* = E(t|y; \theta) \). As \( E(t|x; \theta) = x(W\Sigma_tW^\top + \Psi_e)^{-1}W\Sigma_t \) and \( E(t|y; \theta) = y(C\Sigma_tC^\top + \Psi_f)^{-1}C\Sigma_t \), these components are linear transformations of \( x \) and \( y \) too, but yield different linear sub-spaces than \( x \) and \( y \), respectively, unless \( \Psi_e \) and \( \Psi_f \) are zero matrices (Bach and Jordan, 2005).

Second, we shall stress that the residuals, \( e \) and \( f \) of our model, may be more than simple noise terms. Indeed, they consist of everything that is not in the shared part between \( x \) and \( y \). In particular, \( e \) may contain some signal from additional latent variables specific to \( x \), plus some pure noise. Similarly, \( f \) may contain some signal from additional latent variables specific to \( y \).

Finally, a last remark concerns the computational estimation of the parameters under our model, which is less straightforward than under the original PPLS model. Although we have not fully devised it, additional details on a possible EM algorithm are presented in Appendix D. In particular, the updates in each of the M-steps of the EM for the parameters \( W \) and \( C \) require an optimization problem over the Stiefel Manifold to be solved (Siegel, 2019, Wen and Yin, 2010), while these updates have closed form expressions under the original PPLS model of el Bouhaddani et al. (2017).
3 Simulation study

Now, we present results from two simulation studies aimed to illustrate the limitations of the original PPLS model, and, more precisely, to illustrate the behavior of the estimates for $W$ and $C$ returned by the EM algorithm devised by el Bouhaddani et al. (2017) under the original PPLS model, depending on whether this model is correctly specified or not. For comparison, we further considered estimates returned by the standard (non-probabilistic) PLS-SVD, and the standard PCA (successively applied on the “$x$ and $y$ parts” of the data). The PLS-W2A, which is another symmetrical PLS method that we briefly described in the Introduction (see Rosipal and Krämer (2006), Wegelin (2000), Wold (1985) for more details), was originally considered too. As expected, estimates returned by the PLS-W2A and PLS-SVD methods were very similar under the original PPLS model (because $\text{Var}(xW)$ and $\text{Var}(yC)$ are diagonal under the original PPLS model), but as they were in the second simulation study too, we finally decided to omit their presentation here.

We set the dimensions of the observed sets of variables $x$ and $y$ to $p = q = 20$, the dimension of the sets of latent variables to $r = 3$, and make the sample size vary in $n \in \{50, 250, 500, 1000, 5000\}$. In the first simulation study, we work under the same setting as that considered by el Bouhaddani et al. (2017) in their simulation study. More precisely, data $(X, Y)$ are generated under the original PPLS model, in the particular case where the diagonal elements of both $\Sigma_t$ and $\Sigma_tB^2$ are all distinct. Weight matrices $W$ and $C$ are randomly drawn from the sets of semi-orthogonal matrices of size $p \times r$ and size $q \times r$, respectively, and the diagonal elements of $\Sigma_t$ and $B$ are respectively set to
\( \sigma_i^2 = \exp(-i/5) \) and \( b_i = 1.5 \exp(3(i - 1)/10) \), for \( i \in \{1, 2, 3\} \), just as in [el Bouhaddani et al. (2017)](#). As for the variances of \( e, f \) and \( h \), they are chosen so that the signal-to-noise ratios are equal to 0.25. The main objective of this first study is to empirically confirm that, when the original PPLS model of [el Bouhaddani et al. (2017)](#) is correctly specified, the weights returned by the corresponding EM algorithm are similar to those returned by two PCAs applied on the \( x \) and \( y \) parts of the data. In the second simulation study, data are generated under a model similar to the original PPLS model, except that \( e \) and \( f \) are not of isotropic variance; instead \( e \) and \( f \) are drawn from multivariate Gaussian variables with arbitrary positive semi-definite variance matrices; more precisely, we chose positive-definite matrices ensuring that eigenvectors of matrices \( \text{Var}(x) \) and \( \text{Var}(y) \) were not too close to the left and right singular vectors of \( \text{Cov}(x, y) \) (using a simple acceptance rejection method), to make sure we work under really misspecified models where solutions of the PLS-SVD differ from solutions of two PCAs. The main objective of this second study is to describe how the solutions of the EM algorithm of [el Bouhaddani et al. (2017)](#) behaves when components of maximal covariance are not of respective maximal variances too, that is when the original PPLS model is misspecified. In both studies, the results are computed over 1000 replicates. Results from our simulation studies can be replicated using our R scripts that we will make available on GitHub soon.

Figure 1 presents the median cosine similarity (in absolute values) between the true weights \( W \) and \( C \) and their estimates, computed over 1000 replicates under the original PPLS model (first row), and under our extended PPLS model (second row). Each of the three columns of Figure 1 presents the
results for one particular pair \((W_i, C_i)_{i \in \{1, 2, 3\}}\). Following what et al. (2017) did in their simulation study, we shall stress that the columns of the estimated weight matrices returned by each of the three compared methods were first re-arranged to make sure they matched the ordering of the true weight matrices.

When the PPLS model is correctly specified (top panel of Figure 1), estimates returned by the EM algorithm under the original PPLS models perform similarly to estimates returned by the other PLS techniques (PLS-SVD and PLS-W2A), and they are all reasonably close to the true weight vectors. In particular, their cosine similarity with the true weight vectors tend to 1 as sample size increases. But, as expected, this is also the case for the estimates returned by two PCAs successively applied on \(X\) and \(Y\). This empirically confirms that when the diagonal elements of both \(\Sigma_t\) and \(\Sigma_tB^2\) are all distinct under the original PPLS model, solutions of the PLS-SVD coincide with those of the PCAs (keep in mind that when the diagonal elements of \(\Sigma_t\) and/or \(\Sigma_tB^2\) are not all distinct, solutions of the PLS-SVD still constitute one of the solutions of the PCAs).

On the other hand, when the original PPLS model is misspecified (bottom panel of Figure 1), our results show that, estimates returned by the two PCAs are quite far from the true weight vectors (as expected, by design), while those returned by the PLS-SVD still perform well. As for the EM algorithm devised under the original PPLS model, it performs much worse than the PLS-SVD, and not much better than the two PCAs. To better describe the estimates returned by the EM algorithm devised under the original PPLS model, Figure 2 presents the median cosine similarities (in absolute values)
between these estimates and those returned by the PLS-SVD and the two distinct PCAs. Interestingly, these results show that, on average, estimates returned by the EM algorithm under the original PPLS model are closer to those returned by the PCAs, especially when the original PPLS model is misspecified. Figure 3 in Appendix E further presents the box-plots of the absolute value of the cosine similarities between the estimates returned by the EM algorithm devised under the original PPLS model and those returned by (i) two distinct PCAs, and (ii) the standard PLS-SVD, in our second simulation study (when the original PPLS model is misspecified). These box-plots suggest that, when solutions of the PLS-SVD differ from solutions of two PCAs, estimates returned by the EM algorithm proposed by el Bouhaddani et al. (2017) are generally closer to those returned by the two PCAs. This constitutes a severe limitation for this algorithm: in real-life examples, there is no guarantee that the estimated weight vectors it returns really capture the relationship between $x$ and $y$.

4 Discussion

In this article, we focused on the PPLS model proposed by el Bouhaddani et al. (2017). After highlighting that it corresponds to a probabilistic formulation of PLS-SVD, we showed that the constraints considered in this original PPLS model are too strong: they imply that the weight matrices $W$ and $C$, which are solutions of this original PPLS model, are also necessarily solutions of two distinct PPCA models for $x$ and $y$, respectively. As a result, the original PPLS model defines a very particular subset of distributions for the pair
Figure 1: Median cosine similarities (in absolute values) between the true weight vectors and the estimates returned by (i) the PPLS EM algorithm, (ii) two distinct PCAs on X and Y, and (iii) PLS-SVD on (X, Y). The results are computed over 1000 replicates, for p = q = 20, r = 3 and different sample sizes n ∈ {50, 250, 500, 1000, 5000}. The top panels correspond to the first simulation study where the original PPLS model is correctly specified, while the bottom panels correspond to the second simulation study where the original PPLS model is misspecified.
Figure 2: Median cosine similarities (in absolute values) between the weight vector estimates returned by the EM algorithm devised under the original PPLS model, and those returned by (i) two distinct PCAs on $X$ and $Y$, and (ii) PLS-SVD on $(X, Y)$. The results are computed over 1000 replicates, for $p = q = 20$, $r = 3$ and different sample sizes $n \in \{50, 250, 500, 1000, 5000\}$. The top panels correspond to the first simulation study where the original PPLS model is correctly specified, while the bottom panels correspond to the second simulation study where it is misspecified.
(x, y), under which the two sets of components of maximal covariance are necessarily of respective maximal variances too. This defect severely limits the practical interest of this model.

However, this defect might not be specific to the model proposed by el Bouhaddani et al. (2017). Our results more generally stress that some caution is needed when developing and applying such latent variable models for dimension-reduction: when imposing too strong of constraints on the model parameters, a model whose structural equations seem to correctly describe the relationships between the observed variables, may turn out to be too simplistic. It can define very particular distributions, under which parameters of interest could be obtained under much more simple models. As a result, a close inspection of other probabilistic models might be needed. First consider the case of the Probabilistic PLS Regression (PPLS-R) model proposed by Li et al. (2015). Zheng et al. (2016) already suggested this model shared some similarities with the probabilistic formulation of Principal Component Regression (PPCR) proposed by Ge et al. (2011). As a matter of fact, it seems that the weight matrix in the PPLS-R model proposed by Li et al. (2015) could also be defined from the marginal distribution of the predictors only. Similar concerns may apply to more complex frameworks, such as the mediation analysis, where the objective is to describe the relationships between three sets of variables. For example, Derkach et al. (2019) propose an interesting probabilistic formulation, but it might be worth checking whether the joint distribution of the three sets of variables is really needed to identify their parameters of interest, or whether the constraints they considered are also too strong, and define particular distributions under which these param-
eters can actually be identified using, e.g., the marginal distribution of one particular set of variables.

As shown in the present article, it is sometimes possible to correct for these defects. In the case of the PPLS model originally proposed by el Bouhadani et al. (2017), we were able to relax some of the constraints, and develop a more general probabilistic formulation of the PLS-SVD, under which the joint distribution of \((x,y)\) is generally necessary for the identification of the model parameters. However, the implementation of an EM algorithm for the estimation of the parameters under this extended PPLS model is less straightforward than for the original PPLS model. In particular, each M-step of the algorithm requires a numerical optimization step to update the estimates of the parameters \(W\) and \(C\), whereas such updates are given by closed-form expressions under the original PPLS model. Alternatively, we could propose another version of the model, where parameters \(W\) and \(C\) would not have to be semi-orthogonal matrices. However, for the model to be identifiable, we would have to impose \(\Sigma_t = I_r\) (identifiability would then hold up to an orthogonal transformation for parameters \(W\) and \(C\)), and the corresponding model would actually be the PCCA model proposed by Bach and Jordan (2005).

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Appendices

A Proof of the limitation of the original PPLS model

Here, we prove that the columns of $W$ and $C$, solutions of the original PPLS model, are also necessarily eigenvectors corresponding to the $r$ largest eigenvalues of $\text{Var}(x)$ and $\text{Var}(y)$, respectively.

Under the PPLS proposed by el Bouhaddani et al. (2017) recalled in Equation (1), we have $\text{Var}(x) = W\Sigma_t W^T + \sigma_x^2 I_p$, with $W$ a semi-orthogonal $p \times r$ matrix, $\Sigma_t$ a $r \times r$ diagonal matrix and $W\Sigma_t W^T$ a symmetric $p \times p$ matrix of rank $r < p$. Consider any eigendecomposition $Q\Delta Q^T$ of matrix $W\Sigma_t W^T$: $\Delta$ is then diagonal, with $r$ non-null elements. Moreover, because $W$ is semi-orthogonal and $\Sigma_t$ (square) diagonal (with strictly positive diagonal elements), the $r$ non-null eigenvalues in $\Delta$ are the diagonal elements ($\sigma_1^2, \ldots, \sigma_r^2$) of $\Sigma_t$, and the columns of $W$ are eigenvectors corresponding to these $r$ non-null eigenvalues. Moreover, because $Q$ is orthogonal, we have $\text{Var}(x) = W\Sigma_t W^T + \sigma_x^2 I_p = Q\Delta_2 Q^T$ with $\Delta_2$ the $p \times p$ diagonal matrix with diagonal elements ($\sigma_1^2 + \sigma_x^2, \ldots, \sigma_r^2 + \sigma_x^2, \sigma_x^2, \ldots, \sigma_x^2$). Putting all this together, it follows that the columns of $W$ are eigenvectors of $\text{Var}(x)$ corresponding to its $r$ largest eigenvalues. When the diagonal elements of $\Sigma_t$ are all distinct, the $r$ non-null eigenvalues of $W\Sigma_t W^T$ are of algebraic multiplicity equal to one, and so are the $r$ largest eigenvalues of $\text{Var}(x)$. In this case, the columns of $W$ are the uniquely defined $r$ eigenvectors associated with
the $r$ largest eigenvalues of $\text{Var}(x)$. However, because $(\sigma_{t_1}^2, \ldots, \sigma_{t_r}^2)$ are not necessarily decreasingly ordered, the eigenvectors of $\text{Var}(x)$ associated with the $r$ largest eigenvalues are not necessarily given in the same order as the left singular vectors associated with the $r$ largest singular values of $\text{Cov}(x, y)$.

The PPLS model of el Bouhaddani et al. (2017) also implies that $\text{Var}(y) = C(\Sigma_t B^2 + \sigma_h^2 I_r) C^\top + \sigma_f^2 I_q$, with $C$ a semi-orthogonal $q \times r$ matrix, and $\Sigma_t B^2 + \sigma_h^2 I_r$ a square diagonal matrix of size $r < q$. Arguing as above, it can be shown that the columns of $C$ constitute one particular set of eigenvectors corresponding to the $r$ largest eigenvalues of $\text{Var}(y)$. In particular, when the diagonal elements of $\Sigma_t B^2$ are distinct, the $r$ largest eigenvalues of $\text{Var}(y)$ are of algebraic multiplicity equal to one: the associated eigenvectors are uniquely defined (up to sign), and they correspond to the columns of $C$.

B Additional details for the comparison of the PPCA model given in Equation (2) with the one proposed by Tipping and Bishop (1999)

Consider a matrix $Z$ containing $n \geq 1$ observations of a random variable $z \in \mathbb{R}^d$, $d > 1$. We recall that the principle of the standard PCA applied on $Z$ is to identify a matrix $V$ or $r \leq d$ vectors of weights defining a matrix $\mathcal{Z} = ZV$ of $r$ mutually orthogonal components with maximal variances. The matrix of weights $V$ is then simply given by the eigenvectors associated with
the $r$ largest eigenvalues of the sample variance matrix $Z^\top Z$.

Tipping and Bishop (1999) proposed a probabilistic formulation of PCA, actually inspired by the factor analysis model (Basilevsky, 1994). Their PCCA is defined by the following structural equation

$$z = vA^\top + g,$$  \hspace{1cm} (7)

under the constraints that $v \sim \mathcal{N}(0_r, I_r)$, $g \sim \mathcal{N}(0_d, \sigma^2 I_d)$ and $r < d$. Then, because $\text{Var}(z)$ is the identity matrix, $A$ is only identifiable up to an orthogonal transformation. In addition, because $A$ is not necessarily semi-orthogonal, the $r$ eigenvectors of $AA^\top$ associated with the $r$ largest eigenvalues have first to be computed to retrieve weights similar to those defined in the non-probabilistic PCA framework.

On the other hand, the PCCA model introduced in Section 2.3 is given by the following structural equation

$$z = vV + g,$$  \hspace{1cm} (8)

along with the constraints $v \sim \mathcal{N}(0_r, \Sigma_v)$, $\Sigma_v$ is a $r \times r$ diagonal matrix (with strictly positive diagonal elements), $g \sim \mathcal{N}(0_d, \sigma^2 I_d)$, $V$ is a $d \times r$ semi-orthogonal matrix and $r < d$. Under this model, if the diagonal elements of $\Sigma_v$ are distinct, then the $r$ non-null eigenvalues $\text{Var}(x)$ are distinct, and the columns $V$ are uniquely defined (up to sign) as the associated eigenvectors. On the other hand, if some diagonal elements of $\Sigma_v$ are identical, the eigenvectors associated with the identical eigenvalues are defined only up
to a rotation. In any case, components defined as $zV$ are those (possibly non-uniquely) defined in the non-probabilistic PCA.

Finally, we shall stress that these two models are equivalent, in the following sense. First note that under the setting of Equation (7), $AA^\top$ is of size $d \times d$ and of rank $r < d$, and can then always be decomposed either as $Q\Delta Q^\top$, where $\Delta$ is a $d \times d$ diagonal matrix with strictly positive $r$ first diagonal elements, and $Q$ is a $d \times d$ orthogonal matrix, or as $Q_r\Delta_r Q_r^\top$, with $\Delta_r$ a $r \times r$ diagonal matrix with strictly positive diagonal elements, and $Q_r$ a $d \times r$ semi-orthogonal matrix. Consequently, any solution $A$ of the PPCA model given in Equation (7) defines a solution $V$ of the PPCA model given in Equation (8), with $V = Q_r$ and $\Sigma_v = \Delta_r$. Similarly, for any solution $V$ of the PPCA model given in Equation (8), $A = V\Sigma_v^{1/2}$ is solution of the PPCA model given in Equation (7).

C Proof of the identifiability of the more general probabilistic formulation of PLS-SVD

Our proof is an adaptation of the one presented in el Bouhaddani et al. (2017). Consider two pairs of variables $(x, y)$ and $(\tilde{x}, \tilde{y})$ defined under our extended PPLS model given in Equation (3), with respective parameters sets $\theta = (W, C, \Sigma_c, \Psi_e, \Psi_f)$ and $\tilde{\theta} = (\tilde{W}, \tilde{C}, \tilde{\Sigma}_c, \tilde{\Psi}_e, \tilde{\Psi}_f)$. Denote by $\Sigma$ and $\tilde{\Sigma}$ their variance-covariance matrices. The principle of the proof is to show that
$\Sigma = \tilde{\Sigma}$ implies $\theta = \tilde{\theta}$. So, let us now assume that $\Sigma = \tilde{\Sigma}$, that is

$$W \Sigma_\ell W^T + \Psi_e = \tilde{W} \tilde{\Sigma}_\ell \tilde{W}^T + \tilde{\Psi}_e,$$  \hspace{1cm} (9)

$$C \Sigma_\ell C^T + \Psi_f = \tilde{C} \tilde{\Sigma}_\ell \tilde{C}^T + \tilde{\Psi}_f,$$ \hspace{1.5cm} (10)

$$W \Sigma_\ell C^T = \tilde{W} \tilde{\Sigma}_\ell \tilde{C}^T.$$  \hspace{1cm} (11)

We recall that $W$, $C$, $\tilde{W}$, and $\tilde{C}$ are semi-orthogonal matrices (of respective sizes $p \times r$ and $q \times r$), while $\Sigma_\ell$ and $\tilde{\Sigma}_\ell$ are diagonal matrices (of size $r \times r$) with strictly decreasingly ordered diagonal elements.

First consider Equation (11). $W \Sigma_\ell C^T$ is a $p \times q$ matrix of rank $r$, with $r < \min(p,q)$. Consider any particular singular value decomposition $V \Delta Q^T$ of matrix $W \Sigma_\ell C^T$, with $V$ a square orthogonal matrix of size $p$, $Q$ a square orthogonal matrix of size $q$, and $\Delta$ a rectangular diagonal matrix of size $p \times q$ with $r$ non-null diagonal elements. The columns of $V$ are eigenvectors of $W \Sigma_\ell^2 W^T$, while those of $Q$ are eigenvectors of $C \Sigma_\ell^2 C^T$. Moreover, the diagonal elements of $\Delta$ are the square roots of the eigenvalues of both $W \Sigma_\ell^2 W^T$ and $C \Sigma_\ell^2 C^T$. Then, because $W$ (respectively $C$) is a semi-orthogonal matrix and $\Sigma_\ell$ is diagonal, the columns of $W$ (respectively of $C$) are left (respectively right) singular vectors associated with the $r$ non-null singular values of the matrix $W \Sigma_\ell C^T$, which correspond to the diagonal elements of $\Sigma_\ell$. Moreover, since the diagonal elements of $\Sigma_\ell$ are strictly decreasingly ordered, these $r$ non-null singular values are distinct, and the $r$ associated left and right singular vectors are uniquely defined (up to sign). Similarly, write $\tilde{V} \tilde{\Delta} \tilde{Q}^T$ any particular singular value decomposition of $\tilde{W} \tilde{\Sigma}_\ell \tilde{C}^T$. From the uniqueness of the singular values and of the first $r$ left and right singular vectors (up to
sign), it follows that (i) \( \Delta = \tilde{\Delta} \), (ii) the first \( r \) columns of \( V \) are equal (up to sign) to the first \( r \) columns of \( \tilde{V} \), and (iii) the first \( r \) columns of \( Q \) are equal (up to sign) to the first \( r \) columns of \( \tilde{Q} \). In other words, we have

\[
\begin{align*}
\Sigma_t &= \tilde{\Sigma}_t, \\
W &= \tilde{W}J, \\
C &= \tilde{C}J,
\end{align*}
\]

where \( J \) is a diagonal matrix with ±1 diagonal elements. Then, Equation (9) is equivalent to \( W\Sigma_t W^T + \Psi_e = W\tilde{\Sigma}_t W^T + \tilde{\Psi}_e \), which yields \( \Psi_e = \tilde{\Psi}_e \). In the same way, Equation (10) is equivalent to \( C\Sigma_t C^T + \Psi_f = C\tilde{\Sigma}_t C^T + \tilde{\Psi}_f \), so that \( \Psi_f = \tilde{\Psi}_f \). As a result, the parameters of our extended PPLS model given in Equation (3) are all identifiable (up to sign for the columns of \( W \) and \( C \)).

D Details on an EM algorithm for the estimation of the parameters of the PPLS model given in Equation (3)

As before, we denote by \((X, Y) = ((X_1, \ldots X_n)^\top, (Y_1, \ldots Y_n)^\top)\) the observed sample of \( n \) independent and identically distributed replica of \((x, y)\). On the other hand, we denote by \( T = (T_1, \ldots T_n)^\top \) the \( n \) “observations” of the latent variable \( t \) (which are therefore not observed). To estimate \( \theta = (W, C, \Sigma_t, \Psi_e, \Psi_f) \) from \((X, Y)\), an EM algorithm [Dempster et al., 1977] can
be used, as a closed-form for \( \hat{\theta} \) cannot be obtained by directly maximizing the likelihood of the observed data. The main steps of this EM algorithm are briefly described below, especially to highlight the step that requires an optimization on Stiefel Manifolds.

The observed data likelihood is

\[
L(X, Y; \theta) = \int_T L(X, Y, T; \theta) dT,
\]

where the complete-data likelihood \( L(X, Y, T; \theta) \) is given by

\[
L(X, Y, T; \theta) = \prod_{i=1}^n f(X_i, Y_i, T_i; \theta),
\]

as \( X_i \mid \{ Y_i \mid T_i \}, i \in [1, n] \). Under the extended PPLS model, \( X_i \mid \{ T_i; \theta \} \sim \mathcal{N}(T_iW^\top, \Psi_e) \), \( Y_i \mid \{ T_i; \theta \} \sim \mathcal{N}(T_iC^\top, \Psi_f) \) and \( T_i; \theta \sim \mathcal{N}(0_r, \Sigma_t) \), \( i \in [1, n] \).

Consequently, for any \( i \in [1, n] \), we have

\[
(X_i, Y_i, T_i; \theta) \sim \mathcal{N}
\left(
\begin{pmatrix}
0_{p+q+r}, & W\Sigma_tW^\top + \Psi_e, & W\Sigma_t C^\top, & W\Sigma_t
\end{pmatrix},
\begin{pmatrix}
w\Sigma_t w^\top & C\Sigma_t W^\top & C\Sigma_t C^\top + \Psi_f & C\Sigma_t
\end{pmatrix}.
\right)
\]

Denote by \( \Sigma \) the first \((p+q) \times (p+q)\) block of this variance-covariance matrix.

Then, \( T_i \mid \{ X_i, Y_i \} \) is Gaussian, with \( \mathbb{E}(T_i \mid X_i, Y_i) = (X_i, Y_i)\Sigma^{-1} \begin{pmatrix} W\Sigma_t \\ C\Sigma_t \end{pmatrix} \)
and \( V(T_i | X_i, Y_i) = \Sigma_t - \left( \Sigma_t W^\top, \Sigma_t C^\top \right) \Sigma_t^{-1} \begin{pmatrix} W \Sigma_t \\ C \Sigma_t \end{pmatrix} \). Then \( \mathbb{E}(T_i^\top T_i | X_i, Y_i) = V(T_i | X_i, Y_i) + \mathbb{E}(T_i | X_i, Y_i)^\top \mathbb{E}(T_i | X_i, Y_i) \).

For simplicity, we will use the notation
\[
\mathbb{E}(T_i^\top T_i | X, Y; \theta) = \sum_{i=1}^n \mathbb{E}(T_i^\top T_i | X_i, Y_i; \theta)
\]
\[
\mathbb{E}(T | X, Y; \theta) = \left( \mathbb{E}(T_i | X_i, Y_i; \theta) \right)_{i \in [1,n]}
\]
which are a square matrix of size \( r \), and a \( n \times r \) matrix, respectively.

From any initial value for \( \theta \), the EM algorithm consists in successively iterating two steps, namely the E-step and the M-step. From a value \( \theta^{old} \) for the set of parameters, the conditional moments \( \mathbb{E}(T_i^\top T_i | X, Y, \theta^{old}) \) and \( \mathbb{E}(T | X, Y, \theta^{old}) \) are computed; this is the E-step. Then the M-step consists in updating the values of the parameters, that is finding \( \theta^{new} \), the value of \( \theta \) which maximizes \( \mathbb{E}(\ln(L(X, Y, T; \theta)) | X, Y; \theta^{old}) \). In our case in the M-step, we can successively maximize over \( \theta \) the three following quantities: \( \kappa = \mathbb{E}(\ln(f_{X,T}(X | T; \theta)) | X, Y; \theta^{old}) \), \( \mu = \mathbb{E}(\ln(f_{Y,T}(Y | T; \theta)) | X, Y; \theta^{old}) \) and \( \pi = \mathbb{E}(\ln(f_T(T; \theta)) | X, Y; \theta^{old}) \), which are here given by

\[
\kappa = -\frac{np}{2} \ln(2\pi) - \frac{n}{2} \ln(|\Psi_e|) - \frac{1}{2} \text{Tr}\left( (X^\top X - 2X^\top \mathbb{E}(T | X, Y, \theta^{old}) W^\top \right.
\]
\[
+ W \mathbb{E}(T^\top T | X, Y, \theta^{old}) W^\top \Psi_e^{-1}) \right).
\]

\[
\mu = -\frac{nq}{2} \ln(2\pi) - \frac{n}{2} \ln(|\Psi_f|) - \frac{1}{2} \text{Tr}\left( (Y^\top Y - 2Y^\top \mathbb{E}(T | X, Y, \theta^{old}) C^\top \right.
\]
\[
+ C \mathbb{E}(T^\top T | X, Y, \theta^{old}) C^\top \Psi_f^{-1}) \right).
\]

34
\[ \pi = -\frac{n_r}{2} \ln(2\pi) - \frac{n}{2} \ln(|\Sigma_{ll}|) - \frac{1}{2} \text{Tr} \left( \mathbb{E} \left( \mathbf{T}^\top \mathbf{T} \mid \mathbf{X}, \mathbf{Y}, \theta^{\text{old}} \right) \Sigma_{l}^{-1} \right) . \]

Of course, the updated parameter \( \theta^{\text{new}} \) has to fulfill the constraints of our model. In particular, solutions \( W^{\text{new}} \) and \( C^{\text{new}} \) are defined as the semi-orthogonal matrices \( W \) and \( C \) that maximize \( \kappa \) and \( \mu \) above. More precisely,

\[
W^{\text{new}} = \arg\max_W -\frac{1}{2} \text{Tr} \left( \left( \mathbf{X}^\top \mathbf{X} - 2\mathbf{X}^\top \mathbb{E} \left( \mathbf{T} \mid \mathbf{X}, \mathbf{Y}, \theta^{\text{old}} \right) W^\top + \mathbb{E} \left( \mathbf{T}^\top \mathbf{T} \mid \mathbf{X}, \mathbf{Y}, \theta^{\text{old}} \right) W^\top \right) \Psi_e^{\text{old}-1} \right) \quad \text{s.t.} \quad W^\top W = I_r. \tag{12}
\]

\[
C^{\text{new}} = \arg\max_C -\frac{1}{2} \text{Tr} \left( \left( \mathbf{Y}^\top \mathbf{Y} - 2\mathbf{Y}^\top \mathbb{E} \left( \mathbf{T} \mid \mathbf{X}, \mathbf{Y}, \theta^{\text{old}} \right) C^\top + \mathbb{E} \left( \mathbf{T}^\top \mathbf{T} \mid \mathbf{X}, \mathbf{Y}, \theta^{\text{old}} \right) C^\top \right) \Psi_f^{\text{old}-1} \right) \quad \text{s.t.} \quad C^\top C = I_r. \tag{13}
\]

Under the original and more simple PPLS model, variance matrices \( \Psi_e^{\text{old}} \) and \( \Psi_f^{\text{old}} \) are isotropic, and el Bouhaddani et al. (2017) could derive closed form expressions for \( W^{\text{new}} \) and \( C^{\text{new}} \), by considering Lagrangian functions. However, closed form expressions can not be derived from the Lagrangians in our case, and so optimizations over the Stiefel Manifolds \( \{ W \in \mathbb{R}^{p \times r} \mid W^\top W = I_r \} \) and \( \{ C \in \mathbb{R}^{q \times r} \mid C^\top C = I_r \} \) have to be numerically performed (Siegel, 2019; Wen and Yin, 2010) to update \( W^{\text{new}} \) and \( C^{\text{new}} \) in each M-step of the EM algorithm, which is computationally intensive.
E Additional results under the second simulation study

![Figure 3: Distribution of the absolute values of the cosine similarity between the columns of the weight matrices estimated with the PPLS EM algorithm and the ones obtained via (i) two distinct PCAs on $X$ and $Y$, and (ii) PLS-SVD on $(X,Y)$. The results are computed over 1000 simulations, for $p = q = 20$, $r = 3$, and different sample sizes $n \in \{50, 250, 500, 1000, 5000\}$. The top panels correspond to weights $C$, and the bottom panels correspond to the weights $W$.](image-url)