Probabilistic Rank-One Matrix Analysis with Concurrent Regularization

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Abstract

As a classical subspace learning method, Probabilistic PCA (PPCA) has been extended to several bilinear variants for dealing with matrix observations. However, they are all based on the Tucker model, leading to a restricted subspace representation and the problem of rotational ambiguity. To address these problems, this paper proposes a bilinear PPCA method named as *Probabilistic Rank-One Matrix Analysis* (PROMA). PROMA is based on the CP model, which leads to a more flexible subspace representation and does not suffer from rotational ambiguity. For better generalization, *concurrent regularization* is introduced to regularize the whole matrix subspace, rather than column and row factors separately. Experiments on both synthetic and real-world data demonstrate the superiority of PROMA in subspace estimation and classification as well as the effectiveness of concurrent regularization in regularizing bilinear PPCAs.

1 Introduction

Principal Component Analysis (PCA) [Jolliffe, 2002] is a classical subspace learning technique. It is widely used for various applications such as data compression, computer vision, and pattern recognition. *Probabilistic PCA* (PPCA) [Tipping and Bishop, 1999] is an important extension of PCA. It reformulates PCA as a generative model, which brings two main advantages: 1) It can capture data uncertainty and handle missing values; 2) By introducing proper prior distributions, it enables automatic model selection or incorporation of desired properties such as robustness [Chen *et al.*, 2009], sparsity [Khanna *et al.*, 2015], and large-margin separability [Du *et al.*, 2015]. Although PCA and PPCA have wide applications, they are designed for vector inputs, and require vectorization (reshaping) to deal with multidimensional data. This may lead to some loss of data information due to the broken spatial structures.

To address the above problem, various multilinear extensions of PCA have been proposed, where the input data are represented by *tensors* (multidimensional arrays). Roughly speaking, multilinear PCA methods can be grouped into two branches [Lu *et al.*, 2013]. One is based on the Tucker model [Tucker, 1966] that learns low-dimensional *tensors* from high-dimensional *tensors* [Yang *et al.*, 2004; Ye, 2005; Ye *et al.*, 2004; Xu *et al.*, 2005; Lu *et al.*, 2008]. The other branch is based on the CANDECOMP/PARAFAC (CP) model [Carroll and Chang, 1970; Harshman, 1970] that learns low-dimensional *vectors* from high-dimensional *tensors*, in a *successive* way [Shashua and Levin, 2001; Lu *et al.*, 2009].

Several attempts have also been made to take advantages of both probabilistic models and tensor representations. This paper focuses on *bilinear* extensions of PPCA, which aims to learn a subspace from *matrix* (*second-order tensor*) inputs. Matrix-Variate Factor Analysis (MVFA) [Xie *et al.*, 2008] may be the first bilinear PPCA method. It relates each (matrix) observation to a low-dimensional latent matrix via introducing column and row factor matrices. With the same spirit as MVFA, Probabilistic Second-Order PCA (PSOPCA) [Yu *et al.*, 2011] provides a probabilistic interpretation of bilinear PCAs by assuming that both matrix observations and latent matrices are from *matrix-variate normal distributions* [Gupta and Nagar, 1999]. By adding two extra noise terms to the PSOPCA model, Bilinear Probabilistic PCA (BPPCA) [Zhao *et al.*, 2012] can analytically marginalize out latent matrices and provide closed-form updates for both maximum likelihood estimation (MLE) and maximum a posteriori (MAP) estimation.

All the existing bilinear PPCA methods are *Tucker*-based. They have a *restricted subspace representation* that reuses each column/row factor for constructing multiple bases of the matrix subspace. This enables them to model the matrix subspace with only a small number of parameters, but also limits the flexibility in capturing data characteristics. In addition, like PPCA, Tucker-based PPCAs suffer from *rotational ambiguity* [Tipping and Bishop, 1999; Ahn and Oh, 2003], which means that they can only estimate the span rather than the exact axes of the underlying subspace. This is undesirable for applications such as data interpretation and visualization [Jolliffe, 2002].

To address the above problems of Tucker-based bilinear PPCAs, this paper proposes a bilinear PPCA method based on the CP model, named as **P**robabilistic **R**ank-**O**ne **M**atrix **A**nalysis (PROMA). PROMA models each observation as a linear combination of rank-one matrices, and does not suffer from rotational ambiguity. Moreover, it takes the Tucker-based PPCA model as a special case, providing more flexi-

bility in capturing data characteristics. To obtain robust solutions against overfitting, we need regularization in PROMA. Instead of separately regularizing column and row factors, we propose *concurrent regularization* to penalize the whole matrix subspace and relax the scale restriction of separate regularization, which could lead to better generalization for CP-based PPCAs.

2 Preliminaries

This section describes the notations and definitions needed in the proposed method, and provides a brief review on PPCA and its bilinear extensions.

Notations: Vectors and matrices are denoted by bold lowercase ($\mathbf{x}$) and uppercase ($\mathbf{X}$) letters, respectively. Superscript $\top$ denotes the transposition. Symbols $\otimes$ and $\circledast$ denote the Kronecker and Hadamard (entrywise) product, respectively. $\odot$ is the Khatri-Rao (column-wise Kronecker) product of two matrices $\mathbf{C} = (\mathbf{c}_1, \ldots, \mathbf{c}_P) \in \mathbb{R}^{d_c \times P}$ and $\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_P) \in \mathbb{R}^{d_r \times P}$, which leads to a $d_c d_r \times P$ matrix denoted as $\mathbf{C} \odot \mathbf{R}$ whose pth column is $\mathbf{c}_p \otimes \mathbf{r}_p$ $(p = 1, \ldots, P)$. $\langle \cdot \rangle$ denotes the expectation w.r.t. a certain distribution. $\mathrm{tr}(\cdot)$ is the matrix trace, $\mathrm{vec}(\cdot)$ is the vectorization operator that stacks the columns of a matrix into a single column vector, and $\mathrm{diag}(\cdot)$ is the operator that creates a diagonal matrix from a vector or a vector formed by the diagonal elements of a matrix. $\mathcal{N}_{d_c,d_r}(\mathbf{\Xi}, \mathbf{\Sigma}_c, \mathbf{\Sigma}_r)$ denotes a *matrix-variate normal distribution* with the mean matrix $\mathbf{\Xi}$, covariance matrices $\mathbf{\Sigma}_c \in \mathbb{R}^{d_c \times d_c}$ and $\mathbf{\Sigma}_r \in \mathbb{R}^{d_r \times d_r}$, which is related to the multivariate normal distribution in the following way: $\mathbf{X} \sim \mathcal{N}_{d_c,d_r}(\mathbf{\Xi}, \mathbf{\Sigma}_c, \mathbf{\Sigma}_r)$ if and only if $\mathrm{vec}(\mathbf{X}) \sim \mathcal{N}(\mathrm{vec}(\mathbf{\Xi}), \mathbf{\Sigma}_r \otimes \mathbf{\Sigma}_c)$ [Gupta and Nagar, 1999].

PPCA model: PPCA relates a d-dimensional observation vector $\mathbf{x}$ to a q-dimensional latent vector $\mathbf{z}$ as follows:

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}, \tag{1}$$

where $\mathbf{W} \in \mathbb{R}^{d \times q}$ is the factor loading matrix, $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I})$ represents random noise with variance σ^2, $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ is independent of $\boldsymbol{\epsilon}$, and $\boldsymbol{\mu}$ is the mean vector. In essence, the goal of PPCA is to learn a q-dimensional subspace spanned by the columns of $\mathbf{W}$ from d-dimensional observations. When the observation $\mathbf{X} \in \mathbb{R}^{d_c \times d_r}$ is in the matrix form, we need to vectorize $\mathbf{X}$ first, and then perform PPCA on $\mathrm{vec}(\mathbf{X}) \in \mathbb{R}^{d_c \cdot d_r}$.

Tucker-based bilinear PPCA model: Bilinear PPCA methods such as PSOPCA and BPPCA take matrices as inputs without vectorization. They are all based on the Tucker model, which relates each matrix observation with a *latent matrix*. Specifically, they aim to find a $q_c \cdot q_r$-dimensional subspace by modeling a matrix observation $\mathbf{X}$ as follows:

$$\mathbf{X} = \mathbf{U}^c \mathbf{Z} \mathbf{U}^{r\top} + \mathbf{\Xi} + \mathbf{E}, \tag{2}$$

where $\mathbf{Z} \in \mathbb{R}^{q_c \times q_r}$ is a latent matrix with $\mathbf{Z} \sim \mathcal{N}_{q_c,q_r}(\mathbf{0}, \mathbf{I}, \mathbf{I})$ serving as the low-dimensional representation of $\mathbf{X}$, $\mathbf{\Xi}$ is the mean matrix, and $\mathbf{E} \in \mathbb{R}^{d_c \times d_r}$ is a noise matrix and independent of $\mathbf{Z}$. Each element of $\mathbf{E}$ is an independent identically distributed (i.i.d.) normal random variable with $E_{ij} \sim \mathcal{N}(0, \sigma^2)$, which is also equivalent to $\mathbf{E} \sim \mathcal{N}_{d_c,d_r}(\mathbf{0}, \sigma\mathbf{I}, \sigma\mathbf{I})$ with $\sigma > 0$. $\mathbf{U}^c = (\mathbf{u}_1^c, \ldots, \mathbf{u}_{q_c}^c)$ and $\mathbf{U}^r = (\mathbf{u}_1^r, \ldots, \mathbf{u}_{q_r}^r)$ are the column and row factor matrices, respectively.

Compared with the PPCA model (1), Tucker-based one (2) requires much fewer parameters ($\mathbf{U}^c$ and $\mathbf{U}^r$ rather than $\mathbf{W}$) to model the same number of latent features, while, as will be seen in the next section, this subspace representation is relatively restricted and has limited flexibility in capturing data characteristics.

3 Probabilistic Rank-One Matrix Analysis with Concurrent Regularization

This section presents our **P**robabilistic **R**ank-**O**ne **M**atrix **A**nalysis (PROMA) method in three stages: 1) We introduce a CP-based bilinear PPCA Model, which is more general than the Tucker-based one (2); 2) *concurrent regularization* is proposed to alleviate overfitting for CP-based PPCAs; 3) we develop the PROMA algorithm with a data-dependent strategy of determining the regularization parameter.

3.1 CP-Based Bilinear PPCA Model

We assume that an observed matrix $\mathbf{X}$ can be represented by a linear combination of P rank-one matrices, whose coefficients are the elements of a latent vector $\mathbf{z} \in \mathbb{R}^P$. This leads to a CP model as follows:

$$\mathbf{X} = \sum_{p=1}^{P} z_p \mathbf{c}_p \mathbf{r}_p{}^\top + \mathbf{\Xi} + \mathbf{E} = \mathbf{C}\,\mathrm{diag}(\mathbf{z})\mathbf{R}^\top + \mathbf{\Xi} + \mathbf{E}, \tag{3}$$

where z_p is the pth element of $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, and $\mathbf{E} \sim \mathcal{N}_{d_c,d_r}(\mathbf{0}, \sigma\mathbf{I}, \sigma\mathbf{I})$ with $\sigma > 0$. $\mathbf{C} = (\mathbf{c}_1, \ldots, \mathbf{c}_P) \in \mathbb{R}^{d_c \times P}$ and $\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_P) \in \mathbb{R}^{d_r \times P}$ are the column and row factor matrices, respectively.

Despite of modeling data in different ways, (1), (2), and (3) have the same goal of learning a subspace from $\mathrm{vec}(\mathbf{X})$ or $\mathbf{X}$. In the following discussions, we study different PPCA models in a typical subspace learning setting, where the dimensionality of the matrix subspace or the number of latent features is given, i.e. $q = q_c \cdot q_r = P$.

Connections with PPCA: We first explore the connections between PPCA and its bilinear extensions.

Proposition 1. *Given $q = q_c \cdot q_r = P$, the Tucker and CP models (2) and (3) are equivalent to the PPCA model (1) with $\mathbf{W} = \mathbf{U}^r \otimes \mathbf{U}^c$ and $\mathbf{R} \odot \mathbf{C}$, respectively.*

Proof. By vectorizing both sides of (2) and (3), and using the fact that $\mathrm{vec}(\mathbf{U}^c\mathbf{Z}\mathbf{U}^{r\top}) = (\mathbf{U}^r \otimes \mathbf{U}^c)\mathrm{vec}(\mathbf{Z})$, the Tucker model (2) can be rewritten as follows:

$$\mathrm{vec}(\mathbf{X}) = (\mathbf{U}^r \otimes \mathbf{U}^c)\mathrm{vec}(\mathbf{Z}) + \boldsymbol{\mu} + \boldsymbol{\epsilon}.$$

With $\mathrm{vec}(z_p \mathbf{c}_p \mathbf{r}_p{}^\top) = z_p \mathbf{r}_p \otimes \mathbf{c}_p$, the CP model (3) becomes:

$$\mathrm{vec}(\mathbf{X}) = \sum_{p=1}^{q} z_p \mathbf{r}_p \otimes \mathbf{c}_p + \boldsymbol{\mu} + \boldsymbol{\epsilon} = (\mathbf{R} \odot \mathbf{C})\mathbf{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}.$$

Since $\mathbf{z} = \mathrm{vec}(\mathbf{Z}) \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, $\boldsymbol{\mu} = \mathrm{vec}(\mathbf{\Xi})$, and $\boldsymbol{\epsilon} = \mathrm{vec}(\mathbf{E}) \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I})$, (2) and (3) are equivalent to the PPCA model (1) with $\mathbf{W} = \mathbf{U}^r \otimes \mathbf{U}^c$ for the Tucker model, and $\mathbf{W} = (\mathbf{r}_1 \otimes \mathbf{c}_1, \ldots, \mathbf{r}_P \otimes \mathbf{c}_P) = \mathbf{R} \odot \mathbf{C}$ for the CP model. □

Proposition 1 implies that both the Tucker- and CP-based PPCAs can be viewed as PPCA with a specific parameterization of the factor matrix $\mathbf{W}$. This also means that inferring the Tucker and CP models is equivalent to estimating a subspace spanned by the columns of $\mathbf{U}^r \otimes \mathbf{U}^c$ and $\mathbf{R} \odot \mathbf{C}$, respectively.

Connections with Tucker-based bilinear PPCAs: Next, we will show that in the same setting of subspace learning, the Tucker model (2) is a special case of the CP model (3).

Theorem 1. *Given $P = q_c \cdot q_r$, the Tucker model (2) is a special case of the CP model (3).*

Proof. The Tucker model (2) can be rewritten as the following summation form of the CP model (3):

$$\mathbf{X} = \sum_{i,j=1}^{q_c,q_r} Z_{ij}\mathbf{u}_i^c{\mathbf{u}_j^r}^\top + \mathbf{\Xi} + \mathbf{E} = \hat{\mathbf{C}}\,\mathrm{diag}(\mathbf{z})\hat{\mathbf{R}}^\top + \mathbf{\Xi} + \mathbf{E},$$

where $\mathbf{z} = \mathrm{vec}(\mathbf{Z})$, $\hat{\mathbf{C}} = (\mathbf{u}_1^c, \ldots, \mathbf{u}_1^c, \ldots, \mathbf{u}_{q_c}^c, \ldots, \mathbf{u}_{q_c}^c)$, and $\hat{\mathbf{R}} = (\mathbf{U}^r, \ldots, \mathbf{U}^r)$. Therefore, the Tucker model is just a CP model with q_r and q_c *repeated* $\mathbf{u}_i^c$ $(i = 1, \ldots, q_c)$ and $\mathbf{u}_j^r$ $(j = 1, \ldots, q_r)$ in $\mathbf{C}$ and $\mathbf{R}$, respectively. □

From Proposition 1 and Theorem 1, the Tucker model (2) represents the matrix subspace as $\mathbf{U}^r \otimes \mathbf{U}^c = \hat{\mathbf{R}} \odot \hat{\mathbf{C}} = (\mathbf{u}_1^r \otimes \mathbf{u}_1^c, \mathbf{u}_2^r \otimes \mathbf{u}_1^c, \ldots, \mathbf{u}_{q_r}^r \otimes \mathbf{u}_1^c, \mathbf{u}_1^r \otimes \mathbf{u}_2^c, \ldots, \mathbf{u}_{q_r}^r \otimes \mathbf{u}_{q_c}^c)$. It *reuses* each column of $\mathbf{U}^c$ and $\mathbf{U}^r$ to construct multiple bases of the matrix subspace. This makes each subspace basis constructed by $\mathbf{u}_i^c$ and $\mathbf{u}_j^r$ $(i = 1, \ldots, q_c; j = 1, \ldots, q_r)$ share some common information with $(q_c - 1) + (q_r - 1)$ other bases, leading to restricted flexibility in capturing data characteristics. In contrast, the CP model (3) does not have this restriction and allows each subspace basis $\mathbf{r}_p \otimes \mathbf{c}_p$ to be constructed by *distinct* pair of factors. Thus, it generalizes the Tucker model (2), and has more potential of capturing useful data characteristics.

Log-likelihood function: Armed with the CP model (3), the conditional distribution of $\mathbf{X}$ given $\mathbf{z}$ is as follows:

$$\mathbf{X}|\mathbf{z} \sim \mathcal{N}_{d_c,d_r}(\sum_{p=1}^{P} z_p \mathbf{c}_p \mathbf{r}_p^\top + \mathbf{\Xi}, \sigma\mathbf{I}, \sigma\mathbf{I}), \tag{4}$$

which is also equivalent to $\mathrm{vec}(\mathbf{X})|\mathbf{z} \sim \mathcal{N}((\mathbf{R} \odot \mathbf{C})\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$. Without loss of generality, we assume that data are centered and thus $\mathbf{\Xi} = \mathbf{0}$. Given a set of observations $\{\mathbf{X}_n\}_{n=1}^N$, we can take the expectation of *the complete-data log-likelihood* $\mathcal{L} = \sum_{n=1}^N \ln p(\mathbf{X}_n, \mathbf{z}_n)$ w.r.t. the conditional distribution $p(\mathbf{z}|\mathbf{X})$. Defining the parameter set $\boldsymbol{\theta} = \{\mathbf{C}, \mathbf{R}, \sigma^2\}$, we have

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) = -\sum_{n=1}^{N}\Bigg[&\frac{d_c d_r}{2}\ln\sigma^2 + \frac{1}{2}\langle \mathbf{z}_n^\top \mathbf{z}_n\rangle \\ &+\frac{1}{2\sigma^2}\langle ||\mathbf{X}_n - \mathbf{C}\,\mathrm{diag}(\mathbf{z}_n)\mathbf{R}^\top||_F^2\rangle\Bigg] + \text{const.}\end{aligned} \tag{5}$$

With the above log-likelihood function, we can estimate the model parameters by maximizing (5) w.r.t. $\boldsymbol{\theta}$.

Rotational ambiguity avoided: Apart form its flexibility, another advantage of the CP model over the Tucker one is that it *does not suffer from rotational ambiguity*. This means that maximizing the likelihood function (5) leads to unique $\mathbf{C}$ and $\mathbf{R}$ up to rotation transformations, which results in the optimal *axes* of the matrix subspace in the sense of maximum likelihood. This property could be very useful in data interpretation and visualization. In contrast, Tucker-based bilinear PPCAs have *rotational ambiguity* and can only obtain *arbitrary bases* spanning the subspace, since their solutions with and without rotation transformations are equally good in terms of the likelihood function [Zhao *et al.*, 2012].

3.2 Regularization for CP-based PPCAs

In order to obtain robust solutions against overfitting, it is common to regularize the log-likelihood function (5) by adding certain regularization terms for $\mathbf{C}$ and $\mathbf{R}$ or introducing priori distributions over $\mathbf{C}$ and $\mathbf{R}$ *separately*.

Separate regularization: For clarity, we only discuss L_2 regularization for penalizing smoothness, while similar conclusions can also be drawn for more general regularizations. It would be natural to regularize the log-likelihood function (5) as follows:

$$\tilde{\mathcal{L}}(\boldsymbol{\theta}) = \mathcal{L}(\boldsymbol{\theta}) + \gamma_c \sum_{p=1}^{P} ||\mathbf{c}_p||^2 + \gamma_r \sum_{p=1}^{P} ||\mathbf{r}_p||^2, \tag{6}$$

where γ_c and γ_r are regularization parameters. This is equivalent to introducing Gaussian priori distributions $p(\mathbf{C}|\gamma_c) = \prod_{p=1}^P \mathcal{N}(\mathbf{c}_p|\mathbf{0}, \gamma_c^{-1}\mathbf{I})$ and $p(\mathbf{R}|\gamma_r) = \prod_{p=1}^P \mathcal{N}(\mathbf{r}_p|\mathbf{0}, \gamma_r^{-1}\mathbf{I})$ over the factor matrices $\mathbf{C}$ and $\mathbf{R}$, respectively.

Scale restriction: However, this conventional approach is not good enough for CP-based PPCAs, because $\mathbf{C}$ and $\mathbf{R}$ are penalized *separately*. Recall from Proposition 1 that the CP model learns a subspace spanned by the columns of $\mathbf{W} = \mathbf{R} \odot \mathbf{C}$. Although $\mathbf{W}$ is constructed by $\mathbf{C}$ and $\mathbf{R}$, we eventually favor a smoothed $\mathbf{W}$, whereas imposing smoothness on $\mathbf{C}$ and $\mathbf{R}$ separately may not lead to a smoothed $\mathbf{W}$. Moreover, due to the regularization terms $||\mathbf{c}_p||^2$ and $||\mathbf{r}_p||^2$, (6) restricts the scales of $\mathbf{c}_p$ and $\mathbf{r}_p$ to specific values. However, this restriction seems unnecessary, because (5) is invariant to scale transformations $\mathbf{c}_p \mapsto s\mathbf{c}_p$, $\mathbf{r}_p \mapsto s^{-1}\mathbf{r}_p$ $(s \neq 0)$ and does not prefer certain scales of $\mathbf{c}_p$ and $\mathbf{r}_p$. Consequently, regularizing $\mathbf{C}$ and $\mathbf{R}$ separately may exclude some good solutions in terms of (5). Can we relax such restriction in regularizing CP-based PPCAs?

Concurrent regularization: Bishop [1995] proved that *adding random noise* to the training examples is equivalent to Tikhonov regularization. This inspires us to regularize CP-based PPCAs via introducing additional noise. Instead of generating a noisy training set as [Bishop, 1995], we introduce additional noise by adjusting the noise variance σ^2. Specifically, we *replace* σ^2 in (5) with a regularization parameter γ. Varying the noise level can balance the influences between observations with high likelihood values and those with low ones, which in turn improves robustness against overfitting. In the context of fitting the CP model, the additional noise regularizes $\mathbf{C}$ and $\mathbf{R}$ at the same time. Therefore, we name this strategy *concurrent regularization*.

Unlike separate regularization, concurrent regularization does not restrict the scales of $\mathbf{c}_p$ and $\mathbf{r}_p$. Thus it is more

flexible in regularizing CP-based PPCAs, and has potential to find better solutions. Concurrent regularization can also be viewed as a bias-variance trade-off of the CP model, where we improve the generalization performance by increasing the bias of fitting training data (reflected by γ).

3.3 PROMA Algorithm

This section develops the PROMA algorithm that combines the CP model with concurrent regularization. Note that it is difficult to maximize (5) w.r.t. both $\mathbf{C}$ and $\mathbf{R}$, because they are coupled with each other. To address this problem, we sequentially and conditionally maximizes (5) w.r.t. $\mathbf{C}$ and $\mathbf{R}$ following the expectation-conditional maximization (ECM) approach [Meng and Rubin, 1993]. Specifically, PROMA consists of two steps: the **R**egularized **E**xpectation (RE-step) and the **C**onditional **M**aximization (CM-step).

RE-step: We first evaluate the expectation $\langle \mathbf{z}_n \rangle$ and $\langle \mathbf{z}_n \mathbf{z}_n^\top \rangle$ w.r.t. the conditional distribution $p(\mathbf{z}_n|\mathbf{X}_n)$ (or $p(\mathbf{z}_n|\text{vec}(\mathbf{X}_n))$ equivalently) for each $\mathbf{X}_n$. Using Bayes' rule with $\boldsymbol{\mu} = \text{vec}(\boldsymbol{\Xi}) = \mathbf{0}$, we have

$$\mathbf{z}_n|\text{vec}(\mathbf{X}_n) \sim \mathcal{N}(\mathbf{M}^{-1}\mathbf{W}^\top \text{vec}(\mathbf{X}_n), \gamma\mathbf{M}^{-1}), \quad (7)$$

where $\mathbf{W} = \mathbf{R} \odot \mathbf{C}$, and $\mathbf{M} = \mathbf{W}^\top\mathbf{W} + \gamma\mathbf{I} = \mathbf{C}^\top\mathbf{C} \circledast \mathbf{R}^\top\mathbf{R} + \gamma\mathbf{I}$ is a $P \times P$ matrix. Based on (7), we can compute $\langle \mathbf{z}_n \rangle$ and $\langle \mathbf{z}_n \mathbf{z}_n^\top \rangle$ with the current fixed values of the model parameters as follows:

$$\langle \mathbf{z}_n \rangle = \mathbf{M}^{-1}\text{diag}(\mathbf{C}^\top \mathbf{X}_n \mathbf{R}), \quad (8)$$

$$\langle \mathbf{z}_n \mathbf{z}_n^\top \rangle = \gamma\mathbf{M}^{-1} + \langle \mathbf{z}_n \rangle \langle \mathbf{z}_n \rangle^\top, \quad (9)$$

where γ is the parameter introduced by concurrent regularization, leading to a **R**egularized **E**-step. An appropriate γ regularizes the whole subspace via $\mathbf{W}^\top\mathbf{W} + \gamma\mathbf{I}$, and solves ill-conditioned problems of $\mathbf{M}^{-1}$. This in turn leads to more robust $\langle \mathbf{z}_n \rangle$ and $\langle \mathbf{z}_n \mathbf{z}_n^\top \rangle$ against overfitting.

CM-step: We then maximize the log-likelihood function (5) w.r.t. $\mathbf{C}$ (or $\mathbf{R}$) with the other fixed. By fixing $\mathbf{R}$, we maximize (5) w.r.t. $\mathbf{C}$ and obtain:

$$\tilde{\mathbf{C}} = \left[\sum_{n=1}^{N} \mathbf{X}_n \mathbf{R}\, \text{diag}(\langle \mathbf{z}_n \rangle)\right] \left[\sum_{n=1}^{N} \langle \mathbf{z}_n \mathbf{z}_n^\top \rangle \circledast \mathbf{R}^\top\mathbf{R}\right]^{-1}. \quad (10)$$

With a similar derivation as $\tilde{\mathbf{C}}$, we have

$$\tilde{\mathbf{R}} = \left[\sum_{n=1}^{N} \mathbf{X}_n^\top \tilde{\mathbf{C}}\, \text{diag}(\langle \mathbf{z}_n \rangle)\right] \left[\sum_{n=1}^{N} \langle \mathbf{z}_n \mathbf{z}_n^\top \rangle \circledast \tilde{\mathbf{C}}^\top\tilde{\mathbf{C}}\right]^{-1}. \quad (11)$$

By alternatively iterating between the RE-step and CM-step, we can find the MLE solutions $\hat{\mathbf{C}}$ and $\hat{\mathbf{R}}$. Then the latent representation $\mathbf{z}$ of an observation $\mathbf{X}$ can be computed via $\langle \mathbf{z}|\mathbf{X} \rangle = \mathbf{M}^{-1}\text{diag}(\hat{\mathbf{C}}^\top\mathbf{X}\hat{\mathbf{R}})$. Algorithm 1 is the pseudocode of PROMA. It always increases the log-likelihood function (5) and is guaranteed to converge [Meng and Rubin, 1993].

Connections with Bayesian CP decomposition: Bayesian CP decomposition methods [Xiong *et al.*, 2010; Shan *et al.*, 2011; Zhao *et al.*, 2015] share the same CP model as PROMA, while they focus on *transductive* inferences of estimating the marginal distribution $p(\mathbf{X})$. In contrast, PROMA aims to project high-dimensional data into a low-dimensional subspace, which requires *inductive* inferences of estimating the conditional distribution $p(\mathbf{z}|\mathbf{X})$. Therefore, it is non-trivial to apply Bayesian CP decomposition for subspace learning because $p(\mathbf{z}|\mathbf{X})$ is generally intractable based on Bayesian inference. Moreover, PROMA is equipped with concurrent regularization, while Bayesian CP decomposition methods separately regularize individual factor matrices with priori distributions.

Algorithm 1 Probabilistic Rank-One Matrix Analysis

1: **Input:** Data set $\{\mathbf{X}_n \in \mathbb{R}^{d_c \times d_r}\}_{n=1}^N$, the number of extracted features P, the maximum number of iterations K, and the concurrent regularization parameter γ.
2: Initialize $\mathbf{C}$ and $\mathbf{R}$ randomly, and normalize each column of $\mathbf{C}$ and $\mathbf{R}$ to have unit norm.
3: **repeat**
4: Compute the conditional expectations $\langle \mathbf{z}_n \rangle$ and $\langle \mathbf{z}_n \mathbf{z}_n^\top \rangle$ via (8) and (9), respectively.
5: Update $\mathbf{C}$ and $\mathbf{R}$ via (10) and (11), respectively.
6: **until** convergence or after K iterations.
7: **Output:** The factor matrices $\mathbf{C}$ and $\mathbf{R}$.

Parameter initialization: We use a random scheme to initialize PROMA, where each column of $\mathbf{C}$ and $\mathbf{R}$ is randomly drawn from $\mathcal{N}(\mathbf{0}, \mathbf{I})$. Such initialization puts a random weight on each column of $\mathbf{W} = \mathbf{R} \odot \mathbf{C}$, which will make PROMA favor certain pairs of factors and bias the final results. Thus, the columns of $\mathbf{C}$ and $\mathbf{R}$ are normalized to have *unit norm*, so that the initialized factors are *equally weighted*.

PROMA$^{\text{NR}}$ algorithm: Notice that if σ^2 is still estimated by maximizing the log-likelihood function (5) rather than being replaced by γ, **N**o concurrent **R**egularization is imposed, and we name this algorithm *PROMA^{NR}*. Specifically, maximizing (5) w.r.t. σ^2 leads to

$$\tilde{\sigma}^2 = \frac{1}{Nd_cd_r} \sum_{n=1}^{N} \Big\{ -2\text{tr}\left(\mathbf{X}_n^\top \tilde{\mathbf{C}}\, \text{diag}(\langle \mathbf{z}_n \rangle) \tilde{\mathbf{R}}^\top\right) + \text{tr}\left(\mathbf{X}_n^\top \mathbf{X}_n\right) + \text{tr}\left(\tilde{\mathbf{R}}(\langle \mathbf{z}_n \mathbf{z}_n^\top \rangle \circledast \tilde{\mathbf{C}}^\top\tilde{\mathbf{C}})\tilde{\mathbf{R}}^\top\right) \Big\}. \quad (12)$$

Therefore, PROMA$^{\text{NR}}$ is just PROMA with $\gamma = \sigma^2$ updated according to (12) in each iteration, where σ^2 can be initialized randomly.

Automatic determination of γ: PROMA involves the regularization parameter γ. Cross-validation can be used for parameter determination, while it could be time consuming. Here, we propose a data-dependent strategy to find a reasonably good γ for PROMA. Specifically, we determine γ by performing PROMA$^{\text{NR}}$ with $P = 1$. This provides a one-dimensional search of total data variance captured by the CP model, where data are projected into a one-dimensional subspace. We find this strategy works well empirically, and is also very efficient because PROMA$^{\text{NR}}$ with $P = 1$ is very fast and converges within a few iterations.

4 Experiments

This section evaluates PROMA against competing methods on both synthetic and real-world data sets.

Table 1: Average subspace estimation accuracy of different algorithms on the 2-D synthetic data sets.

Method	PSOPCA	BPPCA	PROMA$^{\text{NR}}$	PROMA
Arc length distance	3.67 $\pm$0.04	3.98 $\pm$0.09	9.70e-8 $\pm$1.46e-8	5.56e-5 $\pm$1.43e-5

4.1 Subspace Estimation on Synthetic Data

We generate synthetic 2-D data sets from the CP model (3) as follows: two factor matrices $\mathbf{C}^*$ and $\mathbf{R}^*$ are generated by drawing each row of $\mathbf{C}^*$ and $\mathbf{R}^*$ from a Gaussian distribution $\mathcal{N}(\mathbf{0}, \mathbf{I}_{P^*})$. Then $N = 1000$ latent vectors $\{\mathbf{z}_n^* \in \mathbb{R}^{P^*}\}_{n=1}^N$ are drawn from $\mathcal{N}(\mathbf{0}, \mathbf{I}_{P^*})$, and the observed matrices with a size of 30×30 are constructed by $\mathbf{X}_n = \mathbf{C}^* \text{diag}(\mathbf{z}_n^*) \mathbf{R}^{*\top}$ *without noise*. According to Proposition 1, the synthetic data lie in the subspace spanned by the columns of $\mathbf{W}^* = \mathbf{R}^* \odot \mathbf{C}^*$. Our aim is to evaluate the subspace estimation accuracy by comparing the *arc length distance* between the estimated subspace $\mathbf{W}$ and the true one $\mathbf{W}^*$. This distance measures the angle between subspaces, and is defined as $||\boldsymbol{\beta}||_2$, where $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_{P^*})$, and $\{\cos(\beta_p)\}_{p=1}^{P^*}$ are the singular values of $\mathbf{W}^\top \mathbf{W}^*$ [Zhao *et al.*, 2012].

We compare PROMA$^{\text{NR}}$, and PROMA ($\gamma = 0.05$) against *Tucker-based PPCAs* including PSOPCA and BPPCA on 10 randomly generated synthetic data sets with $P^* = 9$. PROMA$^{\text{NR}}$ and PROMA with $P = 9$, and PSOPCA and BPPCA with $q_c = 3, q_r = 3$ are performed to estimate the true P^*-dimensional subspace. Table 1 shows the average subspace estimation accuracy of different algorithms. It is clear that PROMA$^{\text{NR}}$ almost perfectly estimates the true subspace, whereas PSOPCA and BPPCA fail to estimate the subspace accurately.

PROMA also gets good results in Table 1 but is worse than PROMA$^{\text{NR}}$, because concurrent regularization introduces additional noise, and reduces the model fit for the ideal data. However, real-world data are usually noisy and not perfectly generated from the CP model. In this case, concurrent regularization, as will be seen, is effective in alleviating overfitting for not only PROMA but also other bilinear PPCAs.

4.2 Classification on Real-World Data

Two face data sets are tested. The first one is a subset of the FERET database [Phillips *et al.*, 2000] including all subjects with at least eight images and at most 15 degrees of pose variation, resulting in 721 face images from 70 subjects.

The second one is a subset from the PIE database [Sim *et al.*, 2003], with seven poses (C05, C07, C09, C27, C29, C37, C11) of at most 45 degrees of pose variation and under 21 illumination conditions (02 to 22). This subset contains 9,987 face images from 68 subjects. Each face image is normalized to 32×32 graylevel pixels.

Algorithms and their settings: We compare PROMA$^{\text{NR}}$ and PROMA against ***linear baselines***: PCA, PPCA; ***Tucker-based PCA***: MPCA [Lu *et al.*, 2008]; ***CP-based PCAs***: TROD [Shashua and Levin, 2001], UMPCA [Lu *et al.*, 2009], and ***Tucker-based PPCAs***: PSOPCA, BPPCA. For completeness, Bayesian CP factorization (BCPF) [Zhao *et al.*, 2015] is also compared, where the conditional expectation of (8) is used to perform dimensionality reduction. We also test PSOPCA and BPPCA with **C**oncurrent **R**egularization as well as PROMA$^{\text{NR}}$ with **S**eparate **R**egularization, denoted by PSOPCA$^{\text{CR}}$, BPPCA$^{\text{CR}}$, and PROMA$^{\text{SR}}$, respectively. We show their best results, where the regularization parameters are selected from $\{10^{-4}, 10^{-3}, \ldots, 10^4\}$.

PCA and MPCA are performed to preserve 97% energy, while changing the value of preserved energy of PCA and MPCA from $95 \sim 99\%$ leads to similar results. For PPCA, UMPCA, PSOPCA, and BPPCA, we test up to 1023, 32, 961, and 961 features, respectively, which are the maximum numbers that can be extracted. We test up to $P = 600$ features for TROD, BCPF, PROMA$^{\text{NR}}$, PROMA$^{\text{SR}}$ and PROMA, since their numbers of extracted feature are not bounded by the input dimensions. For MPCA, TROD, and UMPCA, we use their default settings with up to $1, 10$, and 10 iterations, respectively. BPPCA has both MLE and MAP implementations. We choose the MLE-based one used in face recognition [Zhao *et al.*, 2012] by iterating until convergence. We iterate PROMA$^{\text{NR}}$, PROMA$^{\text{SR}}$, and PROMA until convergence or 500 iterations. The regularization parameter γ of PROMA is automatically determined by PROMA$^{\text{NR}}$ with $P = 1$.

Experiment setup: We randomly split the FERET and PIE data sets into training and test sets so that each subject has L images for training, and the rest are used for test. We report the results over ten such random splits. After feature extraction via each method, all the features are sorted according to the Fisher score [Duda *et al.*, 2012] in descending order, and then the *nearest neighbor classifier* is used to obtain the recognition rates. For each method and L, we report the best recognition rates obtained using different numbers of the extracted features (up to the maximums) in Tables 2 and 3. We highlight the best and comparable results in **bold font** based on t-test with a p-value of 0.01, and underline the second best ones.

Recognition results: Tables 2 and 3 show the recognition results on the FERET and PIE data sets, respectively. PROMA consistently achieves the best results with statistical significance on the whole, while PROMA$^{\text{SR}}$ seems the second best method. PROMA outperforms BPPCA (BPPCA$^{\text{CR}}$), the best Tucker-based PPCA, by 5.44% (3.59%) and 5.13% (4.64%) on average for the FERET and PIE data sets, respectively. This could be attributed to the CP model in characterring the underlying subspace with more flexibility as well as the concurrent regularization in alleviating overfitting. On the other hand, although it already imposes regularization, BCPF does not work well in all the cases, which indicates that applying tensor decomposition methods for subspace learning is not a trivial task.

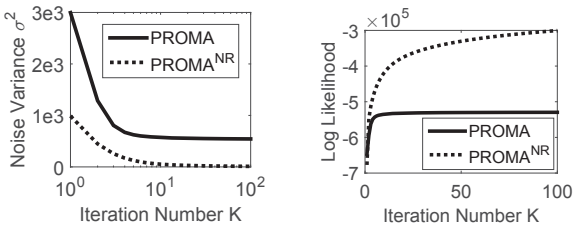
Effectiveness of concurrent regularization: Concurrent regularization significantly improves PROMA$^{\text{NR}}$ by 17.65% and 11.68% on average for the FERET and PIE data sets, respectively. It also improves Tucker-based PPCAs, PSOPCA and BPPCA, in most cases. By optimizing regularized log-likelihood function (6), PROMA$^{\text{SR}}$ always outperforms PROMA$^{\text{NR}}$, while it is still inferior to PROMA. This could be attributed to concurrent regularization in penalizing the whole

Table 2: Recognition rates (Mean±Std.%) on the FERET data set (**Best**; Second best).

L	2	3	4	5	6	7
PCA	46.49±3.43	54.09±4.88	59.71±2.62	67.39±3.36	71.40±2.40	72.16±3.35
PPCA	51.14±1.99	63.78±3.02	69.18±3.44	73.69±0.66	77.94±2.73	77.88±2.79
MPCA	57.56±3.69	67.73±1.87	72.04±2.10	76.60±2.25	79.73±2.55	81.08±2.40
UMPCA	47.72±5.62	57.83±4.18	64.29±3.53	69.87±4.72	73.72±5.08	75.24±2.12
TROD	61.62±2.92	69.49±3.29	74.65±3.00	79.11±1.50	81.89±1.98	83.55±2.26
BCPF	52.67±2.12	62.72±3.24	68.62±2.52	74.04±1.51	77.24±2.42	79.83±2.88
PSOPCA	51.51±2.10	60.47±2.60	65.96±3.04	70.89±2.41	74.49±2.45	75.89±3.17
PSOPCA$^{\text{CR}}$	59.02±2.35	68.18±2.16	72.83±2.66	77.47±1.83	80.20±1.84	81.26±2.39
BPPCA	62.10±3.39	71.06±3.45	76.67±3.34	81.97±1.44	84.52±2.36	85.19±2.13
BPPCA$^{\text{CR}}$	64.30±2.82	73.29±2.25	77.69±2.31	82.35±1.12	84.95±2.19	87.23±2.09
PROMA$^{\text{NR}}$	49.21±2.37	56.99±2.28	62.54±3.59	68.84±1.23	72.52±3.51	75.32±2.41
PROMA$^{\text{SR}}$	64.25±3.25	73.01±2.88	79.09±2.43	83.32±2.64	86.98±2.85	86.54±2.49
PROMA	**67.49±2.59**	**77.16±2.13**	**82.56±3.52**	**85.55±1.82**	**88.84±2.07**	**89.74±2.15**

Table 3: Recognition rates (Mean±Std.%) on the PIE data set (**Best**; Second best).

L	2	3	4	5	6	8	10	20
PCA	26.41±3.35	37.25±1.50	43.04±2.51	49.50±2.14	52.08±2.58	60.68±1.74	66.26±0.87	82.40±0.64
PPCA	24.41±2.14	38.00±0.94	45.48±1.82	51.24±0.93	55.54±0.99	64.25±1.25	69.82±0.48	86.66±3.06
MPCA	35.27±2.97	46.25±2.56	51.74±1.79	56.61±1.63	59.60±0.58	66.75±0.66	71.48±0.66	84.35±1.48
UMPCA	29.08±3.06	38.11±2.11	42.52±3.42	48.34±3.03	51.04±3.05	58.12±3.31	61.61±3.24	76.38±2.39
TROD	34.52±1.84	42.92±2.75	47.90±2.52	52.92±1.87	56.33±1.52	63.30±0.93	67.70±1.21	81.07±1.54
BCPF	31.56±1.13	42.63±1.81	50.00±1.92	57.13±1.79	61.39±0.75	69.55±0.70	74.69±0.60	81.27±1.10
PSOPCA	31.09±3.10	39.21±3.07	45.79±2.98	52.38±2.64	56.60±2.79	63.99±2.41	68.76±2.19	84.37±1.50
PSOPCA$^{\text{CR}}$	35.15±1.23	44.92±1.23	50.61±2.05	56.02±1.16	60.32±1.02	67.77±0.81	71.71±1.16	85.72±0.65
BPPCA	36.07±1.88	47.41±1.93	53.23±2.39	59.25±2.27	63.84±1.81	71.14±1.13	74.83±2.00	88.06±0.95
BPPCA$^{\text{CR}}$	37.39±2.65	47.67±1.91	54.03±2.37	60.53±1.99	63.91±1.88	71.35±2.59	75.09±0.83	87.78±0.94
PROMA$^{\text{NR}}$	27.59±1.12	36.14±1.18	43.86±1.62	51.32±1.39	56.30±1.02	66.07±0.96	72.11±0.64	88.01±1.04
PROMA$^{\text{SR}}$	36.83±1.81	47.82±1.73	55.10±2.03	61.59±1.24	65.47±1.25	72.49±1.18	76.12±0.82	**89.08±0.71**
PROMA	**42.42±1.74**	**53.85±1.71**	**59.91±1.73**	**65.77±1.62**	**69.13±1.27**	**75.28±1.18**	**79.13±0.91**	**89.36±0.67**



(a) Estimated noise variance (b) Log-likelihood

Figure 1: Goodness-of-fit and convergence study for PROMA$^{\text{NR}}$ and PROMA on the FERET data set with $L = 2$.

matrix subspace and relaxing the scale restriction of separate regularization.

Goodness-of-fit: It is worth noting that although PROMA replaces the noise variance σ^2 with the regularization parameter γ, we can still calculate σ^2 for PROMA according to (12), whose value indicates how well the CP model fits the training data. Figure 1(a) shows the noise variance σ^2 of PROMA$^{\text{NR}}$ and PROMA w.r.t. the iteration number K on the FERET data set with $L = 2$. PROMA$^{\text{NR}}$ always has lower noise variance and thus fits the training data better than PROMA, while PROMA consistently achieves much better recognition results than PROMA$^{\text{NR}}$ in Tables 2 and 3. This implies that PROMA$^{\text{NR}}$ suffers from the overfitting problem, whereas PROMA effectively alleviates overfitting via concurrent regularization.

Convergence: Figure 1(b) shows the log-likelihood of PROMA$^{\text{NR}}$ and PROMA at each iteration on the FERET data set with $L = 2$. We can see that PROMA gets lower log-likelihood and converges within a few iterations, while PROMA$^{\text{NR}}$ has higher log-likelihood with slower convergence. This indicates concurrent regularization not only alleviates overfitting but also improves convergence.

5 Conclusion

We proposed a CP-based bilinear PPCA, Probabilistic Rank-One Matrix Analysis (PROMA). Compared with its Tucker-based counterparts, PROMA has a more flexible subspace representation, and does not suffer from rotational ambiguity. For better generalization, we proposed concurrent regularization to penalize the whole matrix subspace and relax the scale restriction of separate regularization. Experiments on both synthetic and real-world data demonstrated the superiority of PROMA in subspace estimation and classification, and also the effectiveness of concurrent regularization in regularizing bilinear PPCAs.

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