Acceleration and Re-start of the Alternating Least Squares Algorithm for Non-linear Principal Components Analysis

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Abstract

In principal components analysis (PCA) of mixture of quantitative and qualitative data, we require to quantify qualitative data. The alternating least squares (ALS) algorithm can be used for PCA including such quantification. However, the ALS algorithm is linear convergence and its speed is very slow in the application of PCA to very large mixed data. In order to circumvent the problem of its slow convergence, Kuroda et al. (2011) provided an acceleration of the ALS algorithm using the vector \( v^e \) algorithm of Wynn (1962). In this paper, we try to further increase the speed of convergence of the \( v^e \) acceleration of the ALS algorithm using a re-starting procedure. Numerical experiments examine how the re-starting procedure works effectively to reduce the number of iterations and computation time of the \( v^e \) acceleration of the ALS algorithm.

Keywords: acceleration of convergence, vector \( v^e \) algorithm, re-starting procedure

1 Introduction

In principal components analysis (PCA) of mixture of quantitative and qualitative data, we require to quantify qualitative data. The PCA including such quantification is called non-linear PCA (Gifi, 1990). The alternating least squares (ALS) algorithm is used as the quantification method and alternates between quantification of qualitative data and computation of ordinary PCA of optimal scaling data. PRINCIPALS of Young et al. (1978) and PRINCALS of Gifi (1990) are popularly used as the ALS algorithm for non-linear PCA. However, the drawback of these algorithms is linear convergence and is very slow in the application of non-linear PCA to very large data. In order to circumvent such slow convergence problem, Kuroda et al. (2011) provided an acceleration method using the vector \( v^e \) algorithm of Wynn (1962). Numerical experiments demonstrated that the \( v^e \) acceleration of the ALS algorithm works well to accelerate the convergence of the sequence generated by the ALS algorithm.

In this paper, we try to re-start the ALS iterations using the \( v^e \) accelerated sequence and generate a new ALS sequence that increases its speed of convergence. The re-starting procedure can reduce the number of iterations and computation time of the \( v^e \) acceleration of the ALS algorithm.

The paper is organized as follows. In Section 2, we present PRINCIPALS used as the ALS algorithm for non-linear PCA and, in Section 3, show the \( v^e \) acceleration of PRINCIPALS (\( v^e \)-PRINCIPALS) that accelerates the convergence of PRINCIPALS. Section 4 proposes a re-starting procedure for speeding up the convergence of PRINCIPALS and describes the procedure of \( v^e \)-PRINCIPALS with the re-starting. Numerical experiments in Section 5 examine the effect of the re-starting for \( v^e \)-PRINCIPALS. In Section 6, we present our concluding remarks.
2 The ALS algorithm for non-linear PCA: PRINCIPALS

Let $X = (X_1 \ X_2 \ \cdots \ X_p)$ be an $n \times p$ matrix of $n$ observations on $p$ variables and be columnwise standardized. In PCA, we postulate that $X$ is approximated by the following bilinear form:

$$\hat{X} = ZA^\top,$$

(1)

where $Z = (Z_1 \ Z_2 \ \cdots \ Z_r)$ is an $n \times r$ matrix of $n$ component scores on $r$ ($1 \leq r \leq p$) components, and $A = (A_1 \ A_2 \ \cdots \ A_r)$ is a $p \times r$ matrix consisting of the eigenvectors of $X^\top X/n$ and $A^\top A = I_r$. Then we determine model parameters $Z$ and $A$ such that

$$\theta = \text{tr}(X - \hat{X})^\top (X - \hat{X}) = \text{tr}(X - ZA^\top)^\top (X - ZA^\top)$$

(2)

is minimized for the prescribed $r$ components.

For observed data being a mixture of quantitative and qualitative data, ordinary PCA cannot be directly applied to such data. Optimal scaling is used to quantify the observed qualitative data and then ordinary PCA can be applied. Let $X^* = (X^*_1 \ X^*_2 \ \cdots \ X^*_p)$ be an $n \times p$ matrix of optimally scaled observations to satisfy restrictions

$$X^{*\top} 1_n = 0_p \quad \text{and} \quad \text{diag} \left[ \frac{X^{*\top} X^*}{n} \right] = I_p,$$

(3)

where $1_n$ and $0_p$ are vectors of ones and zeros of length $n$ and $p$, respectively. In the presence of qualitative data, the optimization criterion (2) is replaced by

$$\theta^* = \text{tr}(X^* - \hat{X})^\top (X^* - \hat{X}) = \text{tr}(X^* - ZA^\top)^\top (X^* - ZA^\top).$$

(4)

In non-linear PCA, we determine the optimal scaling parameter $X^*$, in addition to estimating $Z$ and $A$.

PRINCIPALS

Young et al. (1978) developed PRINCIPALS as the ALS algorithm for non-linear PCA with mixed measurement levels of single nominal, ordinal and numerical variables. PRINCIPALS alternates between ordinary PCA and optimal scaling and finds $X^*$, $Z$ and $A$ by minimizing $\theta^*$ defined by Equation (4) under the restriction (3).

For the initialization of PRINCIPALS, we determine initial data $X^{*(0)}$. The observed data $X$ may be used as $X^{*(0)}$ after it is standardized to satisfy the restriction (3). For given initial data $X^{*(0)}$ with the restriction (3), PRINCIPALS updates each of the parameters $Z$, $A$ and $X^*$ in turn, keeping the others fixed.

- **Model parameter estimation step**: Obtain $A^{(t)}$ by solving

$$\left[ \frac{X^{*(t)\top} X^{*(t)}}{n} \right] A = AD_r,$$

(5)

where $A^\top A = I_r$ and $D_r$ is an $r \times r$ diagonal matrix of eigenvalues, and the superscript $(t)$ indicates the $t$-th iteration. Compute $Z^{(t)} = X^{*(t)} A^{(t)}$. 
• **Optimal scaling step**: Calculate $\hat{X}^{(t+1)} = Z^{(t)} A^{(t)^T}$ from Equation (1). Find $X^{*(t+1)}$ such that

$$X^{*(t+1)} = \arg\min_{X^*} \text{tr}(X^* - \hat{X}^{(t+1)})^T (X^* - \hat{X}^{(t+1)})$$

for fixed $\hat{X}^{(t+1)}$ under measurement restrictions on each of the variables. Scale $X^{*(t+1)}$ by columnwise centering and normalizing.

3 The ηε acceleration of PRINCIPALS: ηε-PRINCIPALS

We briefly introduce the ηε algorithm of Wynn (1962). The ηε algorithm is utilized to speed up the convergence of a slowly convergent vector sequence and is very effective for linearly converging sequences.

Let $\{Y^{(t)}\}_{t=0} = \{Y^{(0)}, Y^{(1)}, Y^{(2)}, \ldots\}$ be a linear convergent sequence generated by an iterative computational procedure. Then the ηε algorithm transforms $\{Y^{(t)}\}_{t=0}^{\infty}$ into another vector sequence $\{Y^{(t')}\}_{t'=0}^{\infty}$ by using

$$Y^{(t')} = Y^{(t)} + \left[\left(Y^{(t'-1)} - Y^{(t)}\right)^{-1} + \left(Y^{(t+1)} - Y^{(t)}\right)^{-1}\right]^{-1},$$

where $[Y]^{-1} = Y/\|Y\|^2$ and $\|Y\|$ is the Euclidean norm of $Y$. When $\{Y^{(t)}\}_{t=0}^{\infty}$ converges to a limit point $Y^{(\infty)}$ of $\{Y^{(t)}\}_{t=0}^{\infty}$, it is known that, in many cases, $\{Y^{(t)}\}_{t=0}^{\infty}$ generated by the ηε algorithm converges to $Y^{(\infty)}$ faster than $\{Y^{(t)}\}_{t=0}^{\infty}$.

We assume that $\{X^{*(t)}\}_{t=0}^{\infty}$ generated by PRINCIPALS converges to a limit point $X^{*(\infty)}$. Then ηε-PRINCIPALS produces a faster convergent sequence $\{X^{*(t')}\}_{t'=0}^{\infty}$ of $\{X^{*(t)}\}_{t=0}^{\infty}$. Given $X^{*(0)}$ and set a desired accuracy $\delta$ for convergence, ηε-PRINCIPALS iterates the following steps:

• **PRINCIPALS step**: Compute $A^{(t)}$ and $Z^{(t)}$ in the Model parameter estimation step and determine $X^{*(t+1)}$ in the Optimal scaling step.

• **Acceleration step**: Calculate $\vec{X}^{*(t-1)}$ using $(X^{*(t-1)}, X^{*(t)}, X^{*(t+1)})$ from

$$\vec{X}^{*(t-1)} = \vec{X}^{*(t)} + \left[\vec{(X^{*(t-1)} - X^{*(t)})}\right]^{-1} + \left[\vec{(X^{*(t+1)} - X^{*(t)})}\right]^{-1},$$

where $\vec{X}^t = (X_1^T X_2^T \ldots X_p^T)^T$. If $||\vec{(X^{*(t-1)} - X^{*(t-2)})}||^2 < \delta$ then stop the algorithm.

Before starting the iteration, we determine initial data $X^{*(0)}$ satisfying the restriction (3) and execute the PRINCIPALS step twice to generate $\{X^{*(0)}, X^{*(1)}, X^{*(2)}\}$.

The ηε acceleration is designed to generate $\{X^{*(t')}\}_{t'=0}^{\infty}$ converging to $X^{*(\infty)}$. Thus the final value of $\{X^{*(t')}\}_{t'=0}^{\infty}$ is the estimate of $X^*$ when ηε-PRINCIPALS terminates. The estimates of $Z$ and $A$ can be calculated immediately from the estimate of $X^*$ in the Model parameter estimation step of PRINCIPALS.

Note that $X^{*(t-1)}$ obtained at the $t$-th iteration of the Acceleration step is not used as the estimate $X^{*(t+1)}$ at the ($t+1$)-th iteration of the PRINCIPALS step. Thus ηε-PRINCIPALS speeds up the convergence of $\{X^{*(t')}\}_{t'=0}^{\infty}$ without affecting the convergence of ordinary PRINCIPALS.
4 The re-starting procedure for \(v\&\)-PRINCIPALS

During the iteration of \(v\&\)-PRINCIPALS, two steps generate two parallel sequences, \(\{X^{(t)}\}_{t}\geq 0\) in the PRINCIPALS step and \(\{X^{*(t)}\}_{t}\geq 0\) in the Acceleration step. We find that \(\{X^{*(t)}\}_{t}\geq 0\) enters rapidly in the neighborhood of \(X^{(\infty)}\). Then, we re-start the iterations of the PRINCIPALS step using a value \(X^{*(t)}\) in \(\{X^{*(t)}\}_{t}\geq 0\) and generate a new sequence \(\{X^{(t)}\}_{t}\geq 0\) that increases its speed of convergence. The rule for re-starting the PRINCIPALS step is given by

\[
|\text{vec}(X^{*(t-1)} - X^{*(t-2)})|^2 \leq \delta_{Re} (> \delta),
\]

and we reset \(\delta_{Re} = \delta_{Re}/K\) at each re-starting, where \(K\) is an integer, such as 10\(^2\). By using the rule (7), we can control the re-starting frequency. For example, let \(\delta = 10^{-12}\), and the initial value of \(\delta_{Re}\) set to 1 and \(K = 10^2\). Then the re-starting procedure is performed at most six times.

When we find a value \(X^{*(t-1)}\) satisfying the condition (7), the re-starting procedure treats \(X^{*(t-1)}\) as the initial value instead of the current estimate \(X^{*(t+1)}\) and the PRINCIPALS step is re-started using \(X^{*(t-1)}\). This re-starting algorithm proposed here is called \(v\&R\)-PRINCIPALS.

For specified \(\delta_{Re}\) and \(K\) in addition to \(X^{*(0)}\) and \(\delta\), \(v\&R\)-PRINCIPALS performs the following steps:

- **PRINCIPALS step:** Compute \(A^{(t)}\) and \(Z^{(t)}\) in the Model parameter estimation step and determine \(X^{*(t+1)}\) in the Optimal scaling step.

- **Acceleration step:** Calculate \(X^{*(t-1)}\) using \(\{X^{*(t-1)}, X^{*(t)}, X^{*(t+1)}\}\) from

\[
\text{vec}X^{*(t-1)} = \text{vec}X^{*(t)} + \left[\text{vec}(X^{*(t-1)} - X^{*(t)})^{-1} + \text{vec}(X^{*(t+1)} - X^{*(t)})^{-1}\right]^{-1}.
\]

If \(|\text{vec}(X^{*(t-1)} - X^{*(t-2)})|^2 < \delta\) then stop the algorithm.

**re-starting:** If \(|\text{vec}(X^{*(t-1)} - X^{*(t-2)})|^2 \leq \delta_{Re}\) then update \(X^{*(t+1)} = X^{*(t-1)}\) and reset \(\delta_{Re} = \delta_{Re}/K\).

5 Numerical experiments

We study how much faster \(v\&R\)-PRINCIPALS converges than PRINCIPALS and \(v\&\)-PRINCIPALS. For all experiments, we set \(\delta = 10^{-12}\) for convergence of \(v\&\)-PRINCIPALS and \(v\&R\)-PRINCIPALS, and terminate PRINCIPALS when \(|\theta^{(t+1)} - \theta^{(t)}| < 10^{-12}\), where \(\theta^{(t)}\) is the \(t\)-th update of \(\theta\) calculated from Equation (4). The maximum number of iterations is set to 10,000. We also specify the initial value of \(\delta_{Re}\) being 1 and \(K = 10^2\) for \(v\&R\)-PRINCIPALS. In this setting, the re-starting procedure performs at most six times. We apply these algorithms to a random data matrix of 100 observations on 15 variables with 10 levels and measure the number of iterations and CPU time taken for \(r = 2\). The procedure is replicated 100 times. All computations are performed with the statistical package \(R\) (R Development Core Team, 2008). CPU times (in seconds) are measured by the function \texttt{proc.time}.

\(^1\)Times are typically available to 10 msec.
Table 1 is summary statistics of the numbers of iterations and CPU times of PRINCIPALS, \(v_e\)-PRINCIPALS and \(v_R\)-PRINCIPALS from 100 simulated data. The table indicates that \(v_e\)-PRINCIPALS and \(v_R\)-PRINCIPALS greatly reduce the number of iterations and CPU time of PRINCIPALS. We also find that, in the case where PRINCIPALS does not converge within 10,000 iterations, two acceleration algorithms still converge. The advantage of these acceleration algorithms is very obvious.

Table 1: Summary of statistics of the numbers of iterations and CPU times of PRINCIPALS (ALS), \(v_e\)-PRINCIPALS (\(v_e\)) and \(v_R\)-PRINCIPALS (\(v_R\)) algorithms from 100 simulated data.

<table>
<thead>
<tr>
<th></th>
<th>The number of iterations</th>
<th>CPU time</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ALS</td>
<td>(v_e)</td>
</tr>
<tr>
<td>Min.</td>
<td>136.0</td>
<td>44.00</td>
</tr>
<tr>
<td>1st Qu.</td>
<td>286.2</td>
<td>94.75</td>
</tr>
<tr>
<td>Median</td>
<td>403.0</td>
<td>122.50</td>
</tr>
<tr>
<td>Mean</td>
<td>598.6</td>
<td>181.76</td>
</tr>
<tr>
<td>3rd Qu.</td>
<td>657.0</td>
<td>183.00</td>
</tr>
<tr>
<td>Max.</td>
<td>10000.0</td>
<td>3326.00</td>
</tr>
</tbody>
</table>

Table 2 is summary statistics of the iteration and CPU time speed-ups for comparing the speed of convergence of PRINCIPALS with that of \(v_e\)-PRINCIPALS and \(v_R\)-PRINCIPALS. The iteration speed-ups are calculated by dividing the number of iterations required for PRINCIPALS by the number of iterations required for \(v_e\)-PRINCIPALS and \(v_R\)-PRINCIPALS, respectively. The CPU time speed-ups are calculated similarly to the iteration speed-up. The table shows that, in mean, \(v_R\)-PRINCIPALS is smaller 5.3 times of iterations and 4.5 times of CPU time than those of PRINCIPALS. We also see that \(v_R\)-PRINCIPALS requires about 2/3 times of the number of iterations and CPU time of \(v_e\)-PRINCIPALS.

Table 2: Summary of statistics of the iteration and CPU time speed-ups of \(v_e\)-PRINCIPALS (\(v_e\)) and \(v_R\)-PRINCIPALS (\(v_R\)) algorithms from 100 simulated data.

<table>
<thead>
<tr>
<th></th>
<th>Iteration speed-up</th>
<th>CPU time speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(v_e)</td>
<td>(v_R)</td>
</tr>
<tr>
<td>Min.</td>
<td>1.832</td>
<td>2.358</td>
</tr>
<tr>
<td>1st Qu.</td>
<td>2.945</td>
<td>4.514</td>
</tr>
<tr>
<td>Median</td>
<td>3.260</td>
<td>5.187</td>
</tr>
<tr>
<td>Mean</td>
<td>3.364</td>
<td>5.281</td>
</tr>
<tr>
<td>3rd Qu.</td>
<td>3.828</td>
<td>5.904</td>
</tr>
<tr>
<td>Max.</td>
<td>5.415</td>
<td>10.842</td>
</tr>
</tbody>
</table>
6 Concluding remarks

In this paper, we provided a re-starting procedure for speeding up the convergence of the \(\psi\)-acceleration of the ALS algorithm. The rule of the re-starting is a very simple and it requires much less computational cost.

Numerical experiments demonstrated that \(\psi\)-R-PRINCALS works effectively to reduce the number of iterations and CPU time of PRINCIPALS and the re-starting procedure works very well to improve the speed of convergence of \(\psi\)-PRINCIPALS. We note that the \(\psi\)-acceleration and the re-starting procedure are applicable to not only PRINCIPALS but also PRINCALS.

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References


