A Constrained Condition-Number LS Algorithm with Its Applications to Reverse Component Analysis and Generalized Oblique Procrustes Rotation

Kohei Adachi

Osaka University, Japan

1. Introduction

1.1 Problem & SVD Reparameterization

1.2 Organization of Presentation

1.1 Problem & SVD Reparameterization

I consider the constrained *LS* problem

$$\text{Min } f(\mathbf{H}) = \|\mathbf{Y} - \mathbf{H}\|^2 \text{ over } \mathbf{H} \text{ s.t. } \underline{CN}(\mathbf{H}) \le u$$

Condition Number *Constant*

For minimizing $f(\mathbf{H})$, I propose to reparameterize $\mathbf{H}$ using its SVD as $\mathbf{H} = a\mathbf{K}\mathbf{\Lambda}\mathbf{L}'$

with $\mathbf{K}'\mathbf{K} = \mathbf{L}'\mathbf{L} = \mathbf{I}_r$, $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_r)$

Then, the problem is reformulated as

$$\text{Min } f(a, \mathbf{K}, \Lambda, \mathbf{L}) = \|\mathbf{Y} - a\mathbf{K}\Lambda\mathbf{L}'\|^2$$
$$\text{over } a, \mathbf{K}, \Lambda, \mathbf{L} \text{ s.t. } 1 \le \lambda_l \le u \quad (l = 1, \ldots, r)$$

1.2 Organization of Presentation

$$\text{Min } f(a, \mathbf{K}, \Lambda, \mathbf{L}) = \|\mathbf{Y} - a\mathbf{K}\Lambda\mathbf{L}'\|^2$$

$$\text{over } a, \mathbf{K}, \Lambda, \mathbf{L}' \text{ s.t. } 1 \le \lambda_l \le u$$

The remaining parts are organized as:

2. Algorithm

for minimizing $f(a, \mathbf{K}, \Lambda, \mathbf{L}')$

3. Simulation Study

for evaluating the algorithm with *reverse component analysis*

4. Application

to generalized oblique Procrustes rotation

5. Conclusion

2. Algorithm

$$\text{Min } f(a, \mathbf{K}, \Lambda, \mathbf{L}) = \|\mathbf{Y} - a\mathbf{K}\Lambda\mathbf{L}'\|^2$$

$$\text{over } a, \mathbf{K}, \Lambda, \mathbf{L}' \quad \text{s.t.} \quad 1 \leq \lambda_l \leq u$$

is attained by alternately iterating the ***a***-, **K**-, **L**- and Λ-**steps** described in the next 2.1 and 2.2

2.1 a-, L-, and K-steps

2.2 Λ-step

2.1 a-, K-, and L-steps

a-Step: min $f(a|\mathbf{K},\Lambda,\mathbf{L}) = ||\mathbf{Y}-a\mathbf{K}\Lambda\mathbf{L}'||^2$ over a

simply attained by **regression without intercept**

L-Step: min $f(\mathbf{L}|a,\mathbf{K},\Lambda) = ||\mathbf{Y}-a\mathbf{K}\Lambda\mathbf{L}'||^2$

over $\mathbf{L}$ s.t. st $\mathbf{L}'\mathbf{L} = \mathbf{I}_r$

K-Step: min $f(\mathbf{K}|a,\Lambda,\mathbf{L}) = ||\mathbf{Y}'-a\mathbf{L}\Lambda\mathbf{K}'||^2$

over $\mathbf{K}$ s.t. st $\mathbf{K}'\mathbf{K} = \mathbf{I}_r$

are equivalent problems attained (explicitly)
by **orthogonal Procrustes rotation**

2.2 Λ-step

$$\min f(\Lambda|a,\mathbf{K},\Lambda,\mathbf{L}) = \|\mathbf{Y}-a\mathbf{K}\Lambda\mathbf{L}'\|^2$$

$$= \|\mathbf{Y}\|^2 + \mathrm{tr}a^2\Lambda^2 - 2\mathrm{tr}\mathbf{Diag}(a\mathbf{L}'\mathbf{Y}'\mathbf{K})\Lambda$$

$$=\|\mathbf{Y}\|^2 + \Sigma_l (a^2\lambda_l^2 - 2d_l\lambda_l)$$

over $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_r)$ s.t. $1 \leq \lambda_l \leq u$

with d_l the (l, l)th element of $a\mathbf{L}'\mathbf{Y}'\mathbf{K}$

attained by finding the λ_l minimizing $a^2\lambda_l^2 - 2d_l\lambda_l$ within $1 \leq \lambda_l \leq u$

$$\lambda_l = \begin{cases} d_l / a^2 & \text{iff } 1 \leq d_l / a^2 \leq u \\ \arg\min_{\lambda_l = 1,u} a^2\lambda_l^2 - 2d_l\lambda_l & \text{otherwise} \end{cases}$$

3. Simulation Study

for assessing how well true matrices are recovered by the proposed algorithm

3.1. Reverse Component Analysis

3.2. Results

3.1 Reverse Component Analysis

[1] Randomly synthesize **true** ${}_{50}\mathbf{H}_{10}$ with $CN(\mathbf{H}) \le 5$

[2] Perform PCA for ${}_{50}\mathbf{H}_{10}$ to obtain its lower rank approximation ${}_{50}\mathbf{F}_q\mathbf{A}_{10}'$ with

$${}_{50}\mathbf{H}_{10} \cong {}_{50}\mathbf{F}_q\mathbf{A}_{10}' \quad (q = 6, \dots, 10)$$

[3] Apply the algorithm for ${}_{50}\mathbf{F}_q\mathbf{A}_{10}'$ for

$$\text{minimizing } f(\mathbf{H}) = \|{}_{50}\mathbf{F}_q\mathbf{A}_{10}' - {}_{50}\mathbf{H}_{10}\|^2 \quad \text{over } \mathbf{H} \text{ s.t. } CN(\mathbf{H}) \le 5$$

This is an attempt to obtain full rank **H** from lower rank **FA**′, and thus ***Reverse*** to ***Principal Component Analysis***.

3.2 Results

I assessed the recovery of $\mathbf{H}_{\mathbf{true}}$ by $\mathbf{H}$ obtained from q-rank approximation ${}_{50}\mathbf{F}_q\mathbf{A}_{10}'$ of $\mathbf{H}_{\mathbf{true}}$, using the index

$$1 - 0.5\|\mathbf{H} - \mathbf{H}_{\mathbf{true}}\|^2 / (\|\mathbf{H} - \mathbf{H}_{\mathrm{ave}}\|^2 + \|\mathbf{H}_{\mathbf{true}} - \mathbf{H}_{\mathrm{ave}}\|^2)$$

with $\mathbf{H}_{\mathrm{ave}}$ containing the average of all elements in $\mathbf{H}$+ $\mathbf{H}_{\mathbf{true}}$

q	**6**	**7**	**8**	**9**	**10**
average	0.944	0.972	0.986	0.995	1.000

The recovery was fairly good, in that the index values average over 500 [$\mathbf{H}$, $\mathbf{H}_{\mathbf{true}}$] were close to **1** (**upper bound**) as shown above.

4. Application

The proposed algorithm is useful for **avoiding** the **degeneration** of solutions in some methods. I illustrate it with the application to **generalized oblique Procrustes rotation**.

4.1 Generalized Oblique Procrustes Rotaton

4.2 Constrained-CN Version

4.1. Generalized Oblique Procrustes Rotation

To match $\mathbf{A}_k\mathbf{T}_k^{-1}$ (**rotated loading matrices**) to $\mathbf{H}$ (**a matrix common across *k***)

$$\text{Min } \ GOPR(\mathbf{T}_k, \mathbf{H}) = \Sigma_k||\mathbf{A}_k\mathbf{T}_k^{-1} - \mathbf{H}||^2$$
$$\text{over } \mathbf{T}_k \text{ and } \mathbf{H} \text{ s.t. } \mathbf{Diag}(\mathbf{T}_k'\mathbf{T}_k) = \mathbf{I}_p$$

However, solutions are known to degenerate with

$$\text{rank}(\mathbf{A}_k\mathbf{T}_k^{-1}) = \text{rank}(\mathbf{H}) = 1.$$

For avoiding the degeneration, we can incorporate constraint $CN(\mathbf{H}) \leq u$ using the propose algorithm.

4.2. Constrained-CN Version

$$GOPR(\mathbf{T}_k,\mathbf{H}) = \Sigma_k \|\mathbf{A}_k\mathbf{T}_k^{-1} - \mathbf{H}\|^2$$

$$= g(\mathbf{T}_k) + K\|\mathbf{A}\mathbf{T} - \mathbf{H}\|^2$$

with $\mathbf{A} = [\mathbf{A}_1, \ldots, \mathbf{A}_K]$, $\mathbf{T} = [\mathbf{T}_1'^{-1}, \ldots, \mathbf{T}_K'^{-1}]'$

Alternating iteration:

min $GOPR(\mathbf{T}_k \mid \mathbf{H})$ over $\mathbf{T}_k$ s.t. $\mathbf{Diag}(\mathbf{T}_k'\mathbf{T}_k) = \mathbf{I}_p$

← **Existing method**

min $\|\mathbf{A}\mathbf{T} - \mathbf{H}\|^2$ over $\mathbf{H}$ s.t. $CN(\mathbf{H}) \le u$

← **Proposed algorithm**

5. Conclusion

5.1 Problem & Algorithm

5.2 Applications

5.1 Problem & Algorithm

For solving the constrained-CN LS problem

$$\min \ f(\mathbf{H}) = \|\mathbf{Y} - \mathbf{H}\|^2 \ \text{ over } \mathbf{H} \text{ s.t. } CN(\mathbf{H}) \le u$$

I proposed an algorithm in which **H** is reparameterized as $a\mathbf{K\Lambda L}'$ to reformulate the problem into

$$\text{Min } \ f(a, \mathbf{K}, \Lambda, \mathbf{L}') = \|\mathbf{Y} - a\mathbf{K\Lambda L}'\|^2$$
$$\text{over } a, \mathbf{K}, \Lambda, \mathbf{L}' \quad \text{s.t.} \quad 1 \le \lambda_l \le u$$

In the algorithm, **regression**, the solving of **quadratic equations**, and **orthogonal Procrustes rotation**, are alternately iterated.

5.2 Applications

The algorithm was evaluated by simulated **Reverse Component Analysis**

$$\min \; f(\mathbf{H}) = \|\mathbf{H}_{\mathbf{reduced}} - \mathbf{H}\|^2 \;\text{ over } \mathbf{H} \text{ s.t. } CN(\mathbf{H}) \leq u$$

with $\mathbf{H}_{\mathbf{reduced}}$ the reduced rank version of $\mathbf{H}_{\mathbf{true}}$, showing the good recovery of $\mathbf{H}_{\mathbf{true}}$ by $\mathbf{H}$.

The constrained condition number algorithm allows **Generalized oblique Procrustes rotation** to **avoid degenerate solutions**.

For an identical purpose, the algorithm could be applied to other analysis procedures.