

A CONTINUOUS-TIME APPROACH TO THE OBLIQUE PROCRUSTES PROBLEM

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In the paper proposed we will make use of the gradient flow approach to consider a generalization of the well-known oblique Procrustes rotation problem, involving oblique simple structure rotation of both the core and component matrices resulting from three-mode factor analysis. The standard oblique Procrustes rotations to specified factor-structure and factor-pattern follow as special cases. The approach adopted leads to globally convergent algorithm and includes solving of initial value problem for certain matrix ordinary differential equation. Necessary conditions are established for the solution of the problem. The same approach is extended easily to the weighted oblique Procrustes rotation. Finally, some simulated numerical results are given and commented.

1. Introduction

Many data analysis problems may be formulated as a matrix fitting problem subject to constraints. Among these, one frequently used model in psychometrics is the so called oblique Procrustes problem (ObPP) (Cox & Cox, 1995 ; Gower, 1984 ; Mulaik, 1972) :

$$\text{minimize } \|AQ - B\|_F \tag{1}$$

$$\text{subject to } \text{diag}(Q^T Q) = I_q. \tag{2}$$

In the above, columns in $Q \in R^{p \times q}$ stand for the direction cosines of q oblique axes in R^p relative to p orthogonal axes and rows of $A \in R^{n \times p}$ standing for n observed points in R^p . Typically, we assume $n \geq p \geq q$. The goal is to select these oblique axes so that rows of the projection AQ are closest to n given points in R^q which are represented by rows in $B \in R^{n \times q}$. In factor analysis the problem (1)-(2) is referred to as oblique Procrustes rotation to the specified factor-structure matrix (containing the covariances/correlations between observed variables and factors). Similarly, the problem

$$\text{minimize } \|AQ^{-T} - B\|_F \tag{3}$$

$$\text{subject to } \text{diag}(Q^T Q) = I_q. \tag{4}$$

is referred to as oblique Procrustes rotation to the specified factor-pattern matrix (containing the weights assigned to the common factors in factor analysis model).

Key Words and Phrases: oblique Procrustes problem, three-mode factor analysis, simple structure rotation, projected gradient flows, optimality conditions

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For details, e.g. (Mulaik, 1972).

A special case of the ObPP with $Q^T Q = I_q$, the so called orthonormal Procrustes problem (OPP), has attracted considerable attention in the literature (Gower, 1984 ; Mulaik, 1972). While the symmetric case $p=q$ of the OPP, also known as the orthogonal Procrustes problem, enjoys a closed-form solution (Golub & Van Loan, 1989 ; Mulaik, 1972), thus far only indirect methods are available for solving the asymmetric OPP ($p > q$). Among these, we mention the Green and Gower iterative algorithm (Gower, 1984), where the asymmetric problem is first embedded into a symmetric problem for which a solution is easy to find, that solution is then used to update the system, and the cycle is repeated. A monotonically decreasing algorithm has been proposed for solving the more complicated weighted OPP in (Mooijaart & Commandeur, 1990 ; Kiers, 1990 ; Koschat & Swayne, 1991 ; Kiers & ten Berge, 1992). Recently in (Chu & Trendafilov, 1998 ; Chu & Trendafilov, submitted) a gradient flow approach has been adopted to solve these problems for which both the symmetric and asymmetric OPP are special cases. The OPP are solved by simply following the integral curve of an ordinary differential equation to the limit point. Its solution can be found by any appropriate ODE numerical integrator (Shampine & Reichelt, 1997). The necessary and the sufficient conditions for both the symmetric and the asymmetric OPP are well understood (Chu & Trendafilov, 1998 ; Chu & Trendafilov, submitted ; Eldén & Park, 1999 ; ten Berge, 1977).

The ObPP (1)-(2), to our knowledge, appears firstly in explicit form in Mosier (1939) where its first approximate solution is given also. The ObPP finds its application in many areas of multivariate data analysis including exploratory factor analysis for common-factor extraction (MINRES) (Mulaik, 1972), maximal degree structure fitting, and various multidimensional scaling techniques (Cox & Cox, 1995 ; Gower, 1984 ; ten Berge, 1991). It also occurs in the context of least squares minimization with a quadratic inequality constraint (Golub & Van Loan, 1989), Section 12.1.

A common feature of the "classical" solutions of the ObPP (1)-(2) is that they take advantage of the fact that the constraint $\text{diag}(Q^T Q) = I_q$ is equivalent to q copies of the unit sphere S^{p-1} in R^p , i.e. the problem can be transformed into q separate problems for each column of Q . The main two approaches to the ObPP differ in using spectral decomposition of $A^T A$ (see Browne, 1967 ; Cramer, 1974) and singular value decomposition of A (see Golub & Van Loan, 1989 ; ten Berge & Nevels, 1977 ; ten Berge, 1991). Both approaches lead to identical secular equations, which in principle, can be solved through the application of any standard root-finding technique, such as Newton's method. The convergence can be very slow and also the iteration can diverge, due to the fact that one solves the equation close to a pole. For solving the secular equation by bidiagonalization of A e.g. (Eldén, 1977). The technique considered further in this work does not rely on solving secular equations. The second ObPP (3)-(4) has been solved columnwise in

(Browne & Kristof, 1969 ; Browne, 1972) by making use of planar rotations and in (Gruvaeus, 1970)—by penalty function approach.

Recently has been found that there are more sophisticated problems involving an oblique rotation where the classical approach can not be applied. Indeed, the problem for oblique simple structure rotation of both the core and component matrices resulting from three-mode factor analysis leads to the following minimization problem (Kiers, 1997) :

$$\begin{aligned} \text{Minimize } & \alpha \|AQ - B\| + \beta \|XQ^{-T} - Y\| & (5) \\ \text{Subject to } & Q \in R^{p \times p}, \text{diag}(Q^T Q) = I_p & (6) \end{aligned}$$

where A, B, X and Y are given matrices of proper dimensions and α and β are known weights. The two extreme cases $\alpha=1, \beta=0$ and $\alpha=0, \beta=1$ simply give the well-known standard ObPP (1)-(2) and (3)-(4) respectively. The problem (5)-(6) can not be solved columnwise, as for the classical ObPP. In the present paper we intend application of the gradient flow approach to solve the problem (5)-(6). The projected gradient approach for solving and analyzing matrix fitting problems involves system of ordinary differential equations (Chu & Driessel, 1990 ; Helmke & Moore, 1994). The idea is that certain numerical method can be though as a discretization of a dynamical system governing a flow that starts at a certain initial state and evolves until it reaches an equilibrium point. By construction it leads to globally convergent algorithms. The method is rather general and can serve as an unified approach for considering least squares data matching problems subject to oblique constraints.

This paper is organized as follows. In Section 2 will be given a formulation of the ObPP in matrix form as a projected gradient flow on the manifold of all square oblique rotations. To make the method presentation less abstract and illustrate how it works we solve (1)-(2) step by step. We start our main task—solving the problem (5)-(6)—in Section 3 with formulation of the three-mode factor analysis model and the problem for simultaneous oblique rotation. The projection technique developed in Section 2 will be applied for solving the problem. As has been told before, its numerical solution can be found by any appropriate ODE numerical integrator. Particularly, we make use of the MATLAB ODE solvers (Shampine & Reichelt, 1997). At the end of the Section we outline briefly how the projected gradient approach can be applied to the following more general problem :

$$\begin{aligned} \text{Minimize } & \alpha \|AQC - B\| + \beta \|XQ^{-T}Z - Y\| & (7) \\ \text{Subject to } & Q \in R^{p \times p}, \text{diag}(Q^T Q) = I_p & (8) \end{aligned}$$

This is an oblique analog of the well-known weighted orthogonal Procrustes problem (known also as Penrose regression problem) (Mooijaart & Commandeur, 1990 ; Koschat & Swayne, 1991 ; Kiers, 1990 ; Kiers & ten Berge, 1992 ; Chu & Trendafilov, 1998). The problem of different weighting of the different dimensions is a special case of (7)-(8). Finally, some simulated numerical results will be given

and commented.

2. Matrix gradient flow approach to ObPP

Here we reconsider the problem (1)-(2) in matrix form. We restrict ourselves to the case when the matrix of oblique rotation Q is square, i.e. $p=q$. The case when $p \neq q$ can be developed by the same manner but is beyond our interest for the aims of the next Section. Let A and B be given matrices. Without loss of generality they can be also assumed $p \times p$ square (follows from the QR decomposition of A and the properties of the Frobenius norm). Consider the function :

$$F(Q) := \frac{1}{2} \langle AQ - B, AQ - B \rangle, \quad (9)$$

where $\langle X, Y \rangle$ denotes the Frobenius inner product of two matrices X and Y and is defined by

$$\langle X, Y \rangle := \text{tr}(XY^T).$$

Consider the smooth manifold $\mathcal{OB}(p)$ of all $p \times p$ oblique rotations, i.e.,

$$\mathcal{OB}(p) := \{Q \in R^{p \times p} : Q^T Q \text{-correlation matrix}\},$$

or simply

$$\mathcal{OB}(p) := \{Q \in R^{p \times p} : \text{diag}(Q^T Q) = I_p\},$$

keeping in mind that every $Q \in \mathcal{OB}(p)$ is nonsingular.

The tangent space $\mathcal{T}_Q \mathcal{OB}(p)$ of this manifold at any $Q \in \mathcal{OB}(p)$ is given by

$$\mathcal{T}_Q \mathcal{OB}(p) = \{H \in R^{p \times p} : \text{diag}(H^T Q + Q^T H) = 0\}.$$

Apparently, the oblique Procrustes rotation problem (1)-(2) is equivalent to the minimization of (9) on the feasible set $\mathcal{OB}(p)$.

By the chain rule and the product rule it is easy to obtain the gradient $\nabla F(Q)$ with respect to the Frobenius inner product of the function $F(Q)$ to be minimized :

$$\nabla F(Q) = A^T(AQ - B). \quad (10)$$

Suppose the projection $g(Q)$ of the gradient $\nabla F(Q)$ onto the tangent space $\mathcal{T}_Q \mathcal{OB}(p)$ can be computed explicitly. Then the differential equation

$$\frac{dQ}{dt} = -g(Q) \quad (11)$$

naturally defines a steepest descent flow for the function F on the feasible set $\mathcal{OB}(p)$. Along the flow $Q(t)$ the function value $F(Q(t))$ is decreasing most rapidly relative to any other direction. Indeed, we have

$$\begin{aligned} \frac{dF(Q)}{dt} &= -\langle \nabla F(Q(t)), g(Q(t)) \rangle \\ &= -\|g(Q(t))\|^2 \end{aligned} \quad (12)$$

due to the fact that $g(Q(t))$ is the orthogonal projection of $\nabla F(Q(t))$ into $\mathcal{T}_{Q(t)}\mathcal{OB}(p)$. It follows from (12) that $F(Q(t))$ is monotonically decreasing function of t . This descent property is universal regardless where the flow starts. Here we give some basic results concerning the convergence properties of the gradient flows. If $Q(t)$ converges to a stationary (or equilibrium) point \bar{Q} , i.e. a point for which $g(\bar{Q})=0$, it follows from (12) that a critical point of F has been reached. Clearly, the convergence of $Q(t)$ to a stationary point is of primary interest for the problem. Denote by

$$\mathcal{E} = \{Q \in \mathcal{OB}(p) : g(Q) = 0\}$$

the set of all stationary points of (11). Then every solution of (11) exists for all $t > 0$ and converges to a compact and connected set that is a subset of \mathcal{E} . Moreover, if the stationary points of g are isolated, then every solution of (11) converges to a single stationary point of g , which is also a critical point for F (12) (Stuart & Humphries, 1996). An example, that convergence to a set (but not to a point) can really happen is constructed in (Palis & de Melo, 1982). Let F is a Morse function, i.e. $F \in C^r$, ($r \geq 2$), (F is continuous together with its r th derivative) and has a finite number of nondegenerate critical points (with nonsingular Hessian). Then $Q(t)$ exists for all $t > 0$ and converges to one of the critical points of F (Hirsh & Smale, 1974; Palis & de Melo, 1982). The above result is also true if the finiteness condition is removed. This, together with the fact that the set of the Morse functions is open and dense in C^r , means that the convergence of $Q(t)$ to a single critical point is a generic property, i.e. the convergence to a set of critical points occurs not “quite often” (Smale, 1960; Helmke & Moore, 1994). Another important feature of the gradient dynamical systems is their structural stability, i.e. any sufficiently small perturbation of the original flow is homeomorphic to the original one. The set of structurally stable gradient vector fields is open and dense in the set of all gradient vector fields, i.e. the structural stability of gradient dynamical systems is generic property (Smale, 1961; Hirsh & Smale, 1974). Particularly, from (12) follows that (11) has no periodic solutions and strange attractors, there is no chaotic behaviour (Peitgen & Richter, 1986).

The core of the method is the construction of the projection of the gradient $\nabla F(Q)$. In the present case this is not a difficult task since $\mathcal{T}_Q\mathcal{OB}(p)$ is explicitly known. The identification of its elements can be found by the well-known fact that any matrix X can be expressed as a sum of its symmetric and skew-symmetric parts, as follows :

$$X = \frac{X + X^T}{2} + \frac{X - X^T}{2}. \tag{13}$$

For our purposes we represent the symmetric part as a sum of a diagonal matrix of the same size composed by its diagonal elements and a symmetric matrix composed by its off-diagonal elements and zero main diagonal. Then for any $p \times$

p matrix the expression (13) can be rewritten as follows :

$$X = \text{off}\left(\frac{X+X^T}{2}\right) + \text{diag}\left(\frac{X+X^T}{2}\right) + \frac{X-X^T}{2}, \quad (14)$$

where for any $p \times p$ matrix X the operator $\text{off}(X)$ is defined as $(\mathbf{1}_p \mathbf{1}_p^T - I_p) \odot X$ and, $\text{diag}(X)$ — as $I_p \odot X$, where \odot denotes the elementwise Hadamard matrix product, $\mathbf{1}_p$ — an $p \times 1$ vector-column of ones and I_p — an $p \times p$ identity matrix.

In this terms the tangent space $\mathcal{T}_Q \mathcal{OB}(p)$ at any $Q \in \mathcal{OB}(p)$ is given by :

$$\begin{aligned} \mathcal{T}_Q \mathcal{OB}(p) &= \{H \in R^{p \times p} : \text{diag}(H^T Q + Q^T H) = 0\} \\ &= \left\{ H : Q^T H = \text{off}\left(\frac{Q^T H + H^T Q}{2}\right) + \frac{Q^T H - H^T Q}{2} \right\} \\ &= \{H : H = Q^{-T}[\text{off}(S) + K]\}, \end{aligned}$$

where S is symmetric and K — skew-symmetric.

It follows that the orthogonal complement of $\mathcal{T}_Q \mathcal{OB}(p)$ in $R^{p \times p}$ with respect to the Frobenius inner product is given by :

$$\mathcal{N}_Q \mathcal{OB}(p) = Q^{-T} D, \text{ for some diagonal } D.$$

In other words we have the following direct-sum representation of $R^{p \times p}$ with respect to the Frobenius inner product :

$$\begin{aligned} R^{p \times p} &= \mathcal{T}_Q \mathcal{OB}(p) \oplus \mathcal{N}_Q \mathcal{OB}(p) \\ &= Q^{-T} \{[\text{off}(S(q)) \oplus S(q)^+] \oplus \mathcal{D}(p)\}, \end{aligned}$$

where

$$\begin{aligned} S(p) &= \{\text{all symmetric } p \times p \text{ matrices}\}, \\ S(p)^+ &= \{\text{all skew-symmetric } p \times p \text{ matrices}\} \end{aligned}$$

and

$$\mathcal{D}(p) = \{\text{all diagonal } p \times p \text{ matrices}\}.$$

Therefore for any $H \in R^{p \times p}$ its projection onto $\mathcal{T}_Q \mathcal{OB}(p)$ has the following unique representation :

$$\pi_{\mathcal{T}_Q \mathcal{OB}(p)}(H) = Q^{-T} \left[\text{off}\left(\frac{Q^T H + H^T Q}{2}\right) + \frac{Q^T H - H^T Q}{2} \right]. \quad (15)$$

Accordingly the projection $g(Q)$ of $\nabla F(Q)$ onto the tangent space $\mathcal{T}_Q \mathcal{OB}(p)$ has the form :

$$\begin{aligned} g(Q) &= \frac{Q^{-T}}{2} [\text{off}(Q^T \nabla F(Q) + \nabla F(Q)^T Q) + (Q^T \nabla F(Q) - \nabla F(Q)^T Q)] \\ &= \frac{Q^{-T}}{2} [\text{off}(2Q^T A^T A Q - Q^T A^T B - B^T A Q) + (B^T A Q - Q^T A^T B)]. \end{aligned} \quad (16)$$

Summarizing, the solution of the ObPP is given by an initial (Cauchy) value problem for the ordinary matrix differential equation

$$\frac{dQ}{dt} = -\frac{Q^{-T}}{2} [\text{off}(2Q^T A^T A Q - Q^T A^T B - B^T A Q) + (B^T A Q - Q^T A^T B)]. \tag{17}$$

and some starting point for the flow. A reasonable starting point for the flow can be the orthonormalized $A^+ B$, where $^+$ is some generalized inverse.

Finally we show that a projected gradient system derived by the projection formulae (15) preserves the flow oblique for all $t > 0$. Indeed, as it has been shown before the general form of the steepest descent flow equation (11) is:

$$dQ/dt = Q^{-T}(\text{off}(S) + K) \tag{18}$$

for some symmetric S and skew-symmetric K . It is easily seen that if $Q(t)$ satisfies (18), then $\text{diag} Q(t)^T Q(t) = I_p$ for $t > 0$. Indeed, noting that

$$d(\text{diag}(Q^T Q))/dt = \text{diag}(d(Q^T Q)/dt) \tag{19}$$

we compute

$$d(Q^T Q)/dt = (dQ/dt)^T Q + Q^T (dQ/dt) = 2\text{off}(S). \tag{20}$$

Thus we have the equation

$$d(\text{diag}(Q^T Q))/dt = 0 \tag{21}$$

and an initial condition $\text{diag}(Q(0)^T Q(0)) = I_p$. From the fundamental existence and uniqueness theorem of the ODE theory (Hirsch & Smale, 1974) one can conclude that the equation (21) leads to $\text{diag}(Q(t)Q(t)^T) = \text{diag}(Q(0)Q(0)^T) = I_p$ for all $t > 0$.

We can derive from the fundamental theory (Gill, Murray, & Wright, 1981), 3.4. a first-order derivative necessary condition for stationary point identification.

Theorem 2.1 *A necessary condition for $Q \in \mathcal{OB}(p)$ to be a stationary point of the square ObPP is that :*

- $B^T A Q \in \mathcal{S}(p)$, i.e. $B^T A Q$ is a symmetric $p \times p$ matrix.
- the off-diagonal elements of the matrix $Q^T A^T A Q$ are equal to those of $B^T A Q$.

Proof. Obviously Q is a stationary point if and only if $g(Q) = 0$. The assertion then follows from (16) since Q is of full rank and the fact that the symmetric and skew-symmetric parts of the projection (16) must zero independently. \square

The first condition in Theorem 2.1 is the well-known necessary condition for orthogonal Procrustes problem derived in (ten Berge, 1977), see also (Chu & Trendafilov, 1998). Our additional second condition is new and reflects the fact we deal with oblique rotations.

3. Oblique simple structure rotation in three-mode factor analysis

We start with a brief outline of the three-mode factor analysis model. Let $Z := \{z_{ijk}\} \in R^{l \times m \times n}$ be a three-mode data matrix, for example, z_{ijk} denotes the observed score of the i th individual ($i = 1, 2, \dots, l$) on the j th variable ($j = 1, 2, \dots, m$) under the k th condition ($k = 1, 2, \dots, m$). For fixed k_0 , we have a matrix composed by $\{z_{ijk_0}\}$,

for $(i=1, 2, \dots, l)$ and $(j=1, 2, \dots, m)$. It is called k_0 th *frontal* slice. Similarly, are defined the i_0 th *horizontal* slice and the j_0 th *lateral* slice. The three-mode factor analysis (Tucker, 1966) can be formulated as a method to seek for representation of the data matrix Z in a form :

$$z_{ijk} = \sum_{\alpha=1}^L \sum_{\beta=1}^M \sum_{\gamma=1}^N c_{\alpha\beta\gamma} g_{i\alpha} h_{j\beta} e_{k\gamma}, \quad (22)$$

where

- $G = \{g_{i\alpha}\} \in R^{L \times L}$, $H = \{h_{j\beta}\} \in R^{m \times M}$ and $E = \{e_{k\gamma}\} \in R^{n \times N}$ are factor-loadings matrices of the “idealized individuals”, “idealized variables” and “idealized conditions” respectively ;
- $C = \{c_{\alpha\beta\gamma}\} \in R^{L \times M \times N}$ is a three-way array called “core” and its elements can be seen as an interaction indicator of the three modes.

Also a matrix formulation of the three-mode factor analysis model (22) in terms of two-mode matrices has been proposed in (Tucker, 1966) :

$$Z_G = GC_G(H^T \otimes E^T), \quad (23)$$

where \otimes denotes the Kronecker matrix product, $Z_G \in R^{l \times mn}$ and $C_G \in R^{L \times MN}$. The $l \times mn$ matrix Z_G is a matrix composed by the frontal slices of the original data matrix Z arranged next to each other. Correspondingly, $L \times MN$ matrix C_G is formed by the frontal slices of the original core array C arranged next to each other. Equivalently we have :

$$Z_H = HC_H(E^T \otimes G^T), \quad (24)$$

$$Z_E = EC_E(G^T \otimes H^T), \quad (25)$$

where $Z_H \in R^{m \times ln}$, $Z_E \in R^{n \times lm}$, $C_H \in R^{M \times LN}$ and $C_E \in R^{N \times LM}$.

In (Tucker, 1966) has been shown that the solution of the three-mode factor analysis is not unique. That is, the factor-loadings matrices G , H , and E can be transformed by any nonsingular matrix which can be compensated by the inverse transformation applied the core, i.e. :

$$Z_G = GC_G(H^T \otimes E^T) = \hat{G} \hat{C}_G (\hat{H}^T \otimes \hat{E}^T), \quad (26)$$

where $\hat{G} = GS^{-T}$, $\hat{H} = HT^{-T}$, $\hat{E} = EU^{-T}$ and $\hat{C}_G = S^T C_G (T \otimes U)$. This freedom in three-mode factor analysis is commonly used to make factor-loadings matrices or/and core array easier to interpret reflecting the factor analysis simple structure concept (Mulaik, 1972). All of the existing methods aim to transform either the factor-loadings matrices or the core array separately. However, when, say, the core is rotated to simple structure this may spoil the simplicity of the factor-loadings matrices and vice versa.

In order to avoid this problem (Kiers, 1997) suggested that oblique simple structure transformation (rotation) should be applied simultaneously on the factor-loadings matrices and the core array. Formally, it leads to solving the following equality constrained optimization problem :

$$\text{Minimize } \alpha \|AQ - B\| + \beta \|XQ^{-T} - Y\| \tag{27}$$

$$\text{Subject to } Q \in R^{p \times p}, \text{diag}(Q^T Q) = I_p \tag{28}$$

where A, B, X and Y are given matrices and α and β are known weights. As it has been said in the beginning of the previous Section the matrices A, B, X and Y can be assumed $p \times p$ square without loss of generality. In this Section the problem (27)-(28) will be considered in details. Consider the function :

$$\begin{aligned} F(Q) &:= F_1(Q) + F_2(Q) \\ &:= \frac{1}{2} \alpha \langle AQ - B, AQ - B \rangle + \frac{1}{2} \beta \langle XQ^{-T} - Y, XQ^{-T} - Y \rangle. \end{aligned} \tag{29}$$

Apparently, the problem (27)-(28) is equivalent to the minimization of (29) on the feasible set $\mathcal{OB}(p)$. The gradients of $F_1(Q)$ and $F_2(Q)$ with respect to the Frobenius inner product are :

$$\nabla F_1(Q) = \alpha A^T (AQ - B) \tag{30}$$

and

$$\nabla F_2(Q) = -\beta Q^{-T} (XQ^{-T} - Y)^T XQ^{-T} \tag{31}$$

correspondingly.

Then the projection $g(Q)$ of $\nabla F(Q)$ onto the tangent space $T_Q \mathcal{OB}(p)$ has the form :

$$\begin{aligned} g(Q) &= \frac{Q^{-T}}{2} \{ \text{off} [2\alpha Q^T A^T A Q - 2\beta Q^{-1} X^T X Q^{-T} \\ &\quad - \alpha(Q^T A^T B + B^T A Q) + \beta(Y^T X Q^{-T} + Q^{-1} X^T Y)] \\ &\quad + \alpha(B^T A Q - Q^T A^T B) + \beta(Y^T X Q^{-T} - Q^{-1} X^T Y) \}. \end{aligned} \tag{32}$$

Correspondingly, the solution of the problem (27)-(28) is given by an initial (Cauchy) value problem for the ordinary matrix differential equation

$$\begin{aligned} \frac{dQ}{dt} &= -\frac{Q^{-T}}{2} \{ \text{off} [2\alpha Q^T A^T A Q - 2\beta Q^{-1} X^T X Q^{-T} \\ &\quad - \alpha(Q^T A^T B + B^T A Q) + \beta(Y^T X Q^{-T} + Q^{-1} X^T Y)] \\ &\quad + \alpha(B^T A Q - Q^T A^T B) + \beta(Y^T X Q^{-T} - Q^{-1} X^T Y) \} \end{aligned} \tag{33}$$

and some starting point for the flow.

We can derive from the fundamental theory (Gill, Murray, & Wright, 1981), 3.4. a first-order derivative necessary condition for stationary point identification.

Theorem 3.1 *A necessary condition for $Q \in \mathcal{OB}(p)$ to be a stationary point of the problem (27)-(28) is that :*

- $\alpha B^T A Q - \beta Q^{-1} X^T Y \in S(p)$, i.e. $\alpha B^T A Q - \beta Q^{-1} X^T Y$ must be a symmetric $p \times p$ matrix ;
- the off-diagonal elements of the matrix $\alpha Q^T A^T A Q - \beta Q^{-1} X^T X Q^{-T}$ must be equal to those of $\alpha B^T A Q - \beta Q^{-1} X^T Y$.

Proof. Obviously Q is a stationary point if and only if $g(Q)=0$. The assertion then follows from (32) since Q is of full rank and the fact that the symmetric and skew-symmetric parts of the projection (32) must zero independently. \square

In case $\alpha=1$ and $\beta=0$ we have precisely the necessary condition known from the previous Section. A necessary condition for factor-pattern Procrustes rotation can be obtained by simply choosing $\alpha=0$ and $\beta=1$.

Finally, at the end of this Section we outline how the projected gradient approach can be applied to the following more complicated oblique Procrustes problem :

$$\text{Minimize } \alpha \|AQC - B\| + \beta \|XQ^{-T}Z - Y\| \quad (34)$$

$$\text{Subject to } Q \in R^{p \times p}, \text{diag}(Q^T Q) = I_p \quad (35)$$

This is an oblique analog of the well-known weighted orthogonal Procrustes problem (known also as Penrose regression problem) (Mooijaart & Commandeur, 1990; Koschat & Swayne, 1991; Kiers, 1990; Kiers & ten Berge, 1992; Chu & Trendafilov, 1998). Indeed, the problem of different weighting of the different dimensions

$$\text{Minimize } \alpha \|(AQ - B)D_c\| + \beta \|(XQ^{-T} - Y)D_z\| \quad (36)$$

$$\text{Subject to } Q \in R^{p \times p}, \text{diag}(Q^T Q) = I_p \quad (37)$$

for given nonnegative diagonal matrices D_c and D_z is special case of (34)-(35).

Consider the function :

$$\begin{aligned} F(Q) &:= F_1(Q) + F_2(Q) \\ &:= \frac{1}{2} \alpha \langle AQC - B, AQC - B \rangle + \frac{1}{2} \langle XQ^{-T}Z - Y, XQ^{-T}Z - Y \rangle. \end{aligned} \quad (38)$$

Apparently, the problem (34)-(35) is equivalent to the minimization of (38) on the feasible set $\mathcal{OB}(p)$. The gradients of $F_1(Q)$ and $F_2(Q)$ with respect to the Frobenius inner product are :

$$\nabla F_1(Q) = \alpha A^T (AQC - B) C^T \quad (39)$$

and

$$\nabla F_2(Q) = -\beta Q^{-T} Z (XQ^{-T} Z - Y)^T X Q^{-T} \quad (40)$$

correspondingly.

Repeating the formalizm described above we arrive at the following matrix ordinary differential equation :

$$\begin{aligned} \frac{dQ}{dt} &= -\frac{Q^{-T}}{2} \{ \text{off} [\alpha (Q^T a Q c + c Q^T a Q) - \alpha (Q^T b + b^T Q) \\ &\quad + \beta (y^T Q^{-T} + Q^{-1} y) - \beta (z Q^{-1} x Q^{-T} + Q^{-1} x Q^{-T} z)] \\ &\quad + \alpha (Q^T a Q c - c Q^T a Q) - \alpha (Q^T b - b^T Q) \\ &\quad + \beta (y^T Q^{-T} - Q^{-1} y) - \beta (z Q^{-1} x Q^{-T} - Q^{-1} x Q^{-T} z) \}, \end{aligned} \quad (41)$$

where $a = A^T A$, $c = C C^T$ and $b = A^T B C^T$, and $x = X^T X$, $z = Z Z^T$ and $y = X^T Y Z^T$.

The flow, starting from some initial value, approximate the solution of (34)-(35).

Theorem 3.2 *A necessary condition for $Q \in \mathcal{OB}(p)$ to be a stationary point of the problem (34)-(35) is that*

$$\alpha Q^T A^T (AQC - B) C^T - \beta Q^{-1} X^T (XQ^{-T} Z - Y) Z^T \quad (42)$$

must be symmetric $p \times p$ matrix.

Proof. Obviously Q is a stationary point if and only if $g(Q) = 0$. The assertion then follows from (41) since Q is of full rank and the fact that the symmetric and skew-symmetric parts of the projection (41) must zero independently. In the present case they both give identical condition. \square

The first term in the necessary condition Theorem 3.2 coincides with the corresponding condition for the weighted orthogonal Procrustes problem derived in (Chu & Trendafilov, 1998). It is easy to check that if C and Z are dropped then we arrive at the result of Theorem 3.1.

4. Numerical experiment

In this section, we report some of our numerical experiments with the equation (33). The computation is carried out by MATLAB 4.2c on an SUN Ultra-2/200 workstation. We choose to use **ode15s** from the MATLAB ODE SUITE (Shampine & Reichelt, 1997) as the integrator for the initial value problems. These codes are available from the network. The code **ode15s** is a quasi-constant step size implementation of the Klopfenstein-Shampine family of the numerical differential formulas (implicit) for stiff systems. More details of these codes can be found in the document (Shampine & Reichelt, 1997).

In our experiments, the tolerance for both absolute error and relative error is set at 10^{-12} . This criterion is used to control the accuracy in following the solution path. The high accuracy we required here has little to do with the dynamics of the underlying vector field, and perhaps is not needed for practical applications in data analysis. It is used only for illustration to accurately follow the flow. Lower accuracy requirement in the calculation certainly can save some CPU time, but not significantly since our calculation is fast already. The output values at time interval of 10 are examined. The integration terminates automatically when the relative improvement of $F(Q)$ between two consecutive output points is less than 10^{-10} , indicating local minimizer has been found. This stopping criterion can be modified if desires to do so.

We should make one more comment concerning the implementation. Note that in theory the flows defined by (33) should automatically stay on the manifold $\mathcal{OB}(p)$. In numerical calculation, however, round-off errors and truncations errors can easily throw the computed $Q(t)$ off the constraint manifold. This can be remedied by replacing $Q(t)$ by the closest oblique rotation in least squares sense

(Section 2 and 3), or simply by

$$\tilde{Q}(t) = Q(t) \text{diag}(\text{diag}(Q(t)'Q(t))^{-1/2}). \quad (43)$$

We have experimented with many tests where the problem data are generated randomly. Because of the global convergence property of our method, all tests have similar dynamical behavior. So as to fit the data comfortably in the running text, we display all numbers only with five digits. All codes used in this experiment are available upon request.

The simulation is organized as follows. We assume $\alpha=1$ and $\beta=1$. We generate uniformly distributed matrices A and X by **rand**(p) and a matrix Q by **rand**(p). After rescaling Q as in (43) it becomes an oblique rotation and we denote it by Q_{in} . Then we define $B=AQ_{\text{in}}$ and $Y=AQ_{\text{in}}^{-T}$ so that the underlying problem has a global solution at Q_{in} . We form initial value for the flow by adding random matrix Q_0 to Q_{in} and rescaling the perturbed matrix Q_0 , i.e.:

$$Q_0 := Q_{\text{in}} + Q_0; \quad Q_0 := Q_0 \text{diag}(\text{diag}(Q_0'Q_0)^{-1/2}); \quad (44)$$

and thus Q_0 is the oblique initial value for the particular problem. We use random matrices with uniformly distributed elements and normally distributed elements with mean 0 and variance 1. The idea of the experiment is to find out how frequently the method proposed is capable to reconstruct Q_{in} starting with random initial Q_0 .

Firstly, we report 100 numerical solutions of the problem (27)-(28) obtained by solving the equation (33). The results presented here are for $p=3$, and 100 perturbations Q_0 . For Q_0 generated by **rand**, the results obtained are as follows: in 62 cases a perfect reconstruction of Q_{in} is found; in 21—the solution deviates considerably from Q_{in} ; in the rest 17 cases no solution is produced for certain CPU time. Total number of flops for all 100 runs is 389464278. For Q_0 generated by **randn**, the results obtained are: in 41 cases a perfect reconstruction of Q_{in} is found; in 34—the solution deviates considerably from Q_{in} ; in the rest 25 cases no solution is produced for certain CPU time. Total number of flops for all 100 runs is 488098461. The difference is easily understandable. It is caused by the fact that the random perturbations generated by **randn** produce initial values Q_0 more deviating from the supposed global solution Q_{in} than those ones generated by **rand**.

Secondly, we give in details a numerical solution of the problem (27)-(28) based on the equation (33) for $p=4$. The following example represent a typical run although the length it takes to reach convergence may vary from data to data. Consider the case where we generate by **rand**:

$$A = \begin{bmatrix} 0.9772 & 0.7433 & 0.9397 & 0.1238 \\ 0.4677 & 0.2053 & 0.9649 & 0.5263 \\ 0.3291 & 0.1714 & 0.2550 & 0.1601 \\ 0.4459 & 0.3725 & 0.0703 & 0.5177 \end{bmatrix},$$

$$X = \begin{bmatrix} 0.1052 & 0.3272 & 0.7582 & 0.9352 \\ 0.8416 & 0.7135 & 0.8366 & 0.6056 \\ 0.3686 & 0.5768 & 0.6998 & 0.3621 \\ 0.4239 & 0.8719 & 0.3891 & 0.5395 \end{bmatrix},$$

and

$$Q_{\text{in}} = \begin{bmatrix} 0.6914 & 0.5987 & 0.1819 & 0.7349 \\ 0.6103 & 0.6708 & 0.6741 & 0.2074 \\ 0.3653 & 0.4115 & 0.4433 & 0.6055 \\ 0.1262 & 0.1491 & 0.5621 & 0.2244 \end{bmatrix}.$$

Then we compute

$$B = \begin{bmatrix} 1.4883 & 1.4888 & 1.1650 & 1.4690 \\ 0.8677 & 0.8933 & 0.9471 & 1.0886 \\ 0.4455 & 0.4407 & 0.3784 & 0.4676 \\ 0.6267 & 0.6230 & 0.6544 & 0.5637 \end{bmatrix}.$$

and

$$Y = \begin{bmatrix} -0.5783 & -0.9428 & 1.6231 & 1.0536 \\ 0.5573 & -0.4456 & 0.7519 & 0.7978 \\ -2.8275 & 3.0091 & 0.2193 & 0.6562 \\ 1.7693 & -1.2351 & 1.0236 & -0.3351 \end{bmatrix}.$$

After perturbing Q_{in} we start from the following oblique matrix :

$$Q_0 = \begin{bmatrix} 0.6022 & 0.5565 & 0.3625 & 0.6241 \\ 0.5645 & 0.5898 & 0.5889 & 0.3786 \\ 0.4508 & 0.4700 & 0.4827 & 0.5638 \\ 0.3398 & 0.3488 & 0.5374 & 0.3865 \end{bmatrix}$$

and we find that the flow $Q(t)$ converges to the oblique matrix

$$Q_{\text{out}} = \begin{bmatrix} 0.6914 & 0.5987 & 0.1819 & 0.7349 \\ 0.6103 & 0.6708 & 0.6741 & 0.2074 \\ 0.3653 & 0.4115 & 0.4433 & 0.6055 \\ 0.1262 & 0.1491 & 0.5621 & 0.2244 \end{bmatrix}.$$

Figure 1 records the history of the changes of the objective value $F(Q(t)) = \alpha \|AQ(t) - B\| + \beta \|XQ(t)^{-T} - Y\|$ where $Q(t)$ is determined by integrating the differential equation (33). Clearly, the global solution is obtained in this case, i.e. the input value Q_{in} is reconstructed completely (Q_{out}). It is easy to check that Q_{out} fulfills the Theorem 3.1.

Also recorded in Figure 1 is the history of the function

$$\Omega(Q(t)) := \|I_p - \text{diag}(Q(t)^T Q(t))\| \tag{45}$$

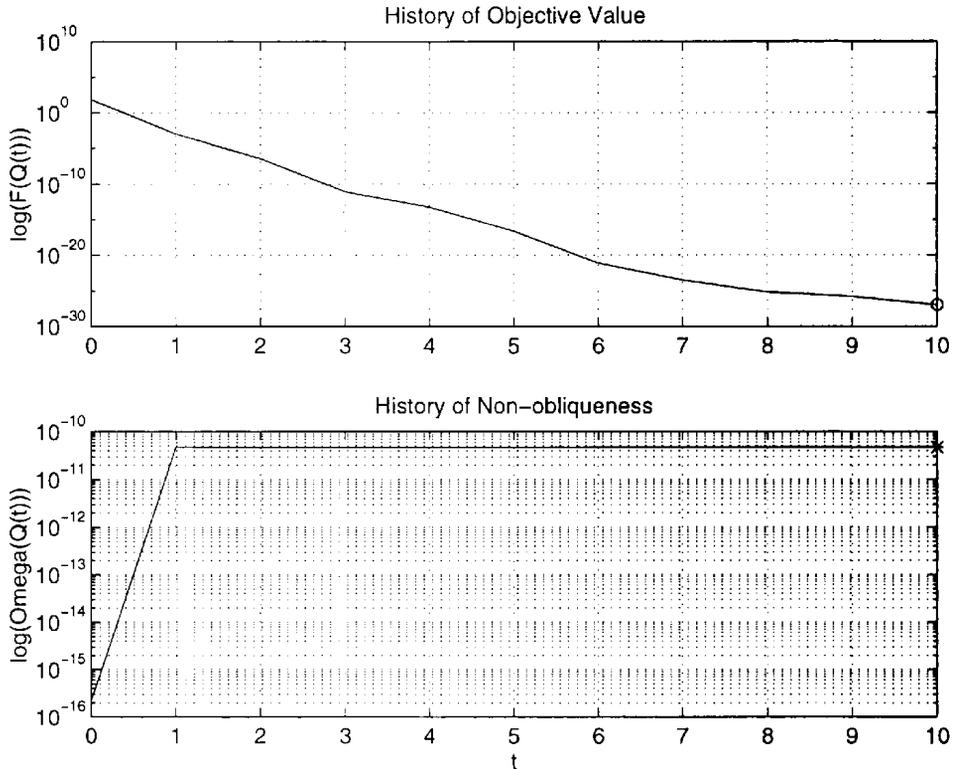


Fig. 1 A semi-log plot of $F(Q(t))$ and $\Omega(Q(t))$ with global minimizer

that measures the deviation of $Q(t)$ from the manifold of constraint $\mathcal{OB}(p)$. It is seen that $Q(t)$ is well kept within the local tolerance.

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